

Bounce Stick Modelling for Particulate Deposition in Gas Turbines



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For Mum, Dad, Mini & Chips.

Abstract

Particulate deposition causes significant damage to gas turbine components, affecting engine performance and incurring substantial maintenance costs. Accurate modelling of deposition enables the likelihood of engine survival in harsh environments to be predicted. For lower levels of deposition it allows maintenance intervals to be determined and the design of components to be made less susceptible to deposition damage.

Modelling deposition requires accurate transport models both of the arrival of particles at vulnerable surfaces and their bounce stick interactions. While there have been considerable advances in transport modelling, bounce stick models have previously failed to capture many physical phenomena robustly. In this thesis a new bounce stick model is reported, particularly suited to the secondary air system of gas turbines.

Bounce stick models are an essential component in deposition modelling as they govern particle interactions with the surface: whether they bounce, stick or shatter upon impact. They also predict the particle rebound trajectory which is particularly important in secondary air system analysis where particles may impinge on multiple surfaces. Existing bounce stick models do not predict particle coefficients of restitution with sufficient accuracy, with notable deficiencies in the modelling of tangential rebound and particle rotation.

A novel bounce stick model based on the analytically-explicit Discrete Element Method (DEM) is proposed in this thesis. The model differs from other models in the literature which are energy-based by explicitly modelling the forces acting on the particles. Furthermore, particular emphasis has been placed on using known (or easily determinable) thermo-mechanical properties of the substrate and particulates with minimal empirical fitting. This should allow the model to be applied to novel material types in future. The modelling framework should allow further development to include features such as particle melt at minimal overhead.

The physics-based DEM model incorporates all first-order physical phenomena relevant to particle deposition in a gas turbine secondary air system. The model was used to predict particle deposition in a number of simple test cases. These allowed the sensitivity of the particle bounce or stick to non-sphericity to be assessed deterministically for the first time. A series of experimentally-validated finite element analysis simulations were used to validate this behaviour.

Another phenomenon which is usually neglected is collision-induced particle rotation (CIR). Here modelling shows that the Magnus force this induces in the surface boundary layer has a non-negligible affect on particle trajectory post-collision, which is particularly significant for particles in closed ducts.

The model has been validated using a unique experimental data set representative of a gas turbine blade cooling passage. A method of implementing the model in a commercial computational fluid dynamics (CFD) code was developed. Excellent qualitative agreement of spatial deposition distribution was achieved in comparison to all other models available in the literature. The method of implementation in CFD includes the modelling of surface roughness and predictions of particle orientation and angular velocity at impact. Numerical predictions confirm the earlier conclusion that CIR and the Magnus force can alter the qualitative and quantitative trends of deposition. With CIR enabled, the approach is able to provide good qualitative predictions of deposition distribution throughout the domain.

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However, the professional and academic achievements of the past few years would cease to have meaning without the friendships and relationships built along the way. Housemates Caleb and Mathilde ensured my sanity throughout the pandemic, whilst Leo's calming Germanic influence subsequently made working from home so enjoyable. The very different distractions provided by the St. Peter's College Boat Club, Liam and many other friends undoubtedly slowed my academic progress by several months. Yet they are truly what have made these near three years worthwhile. Most importantly, the extent to which Lewys has both tolerated and supported me cannot be understated.

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Nomenclature

Abbreviations

CRW	Continuous Random Walk
CV	Critical Velocity
DEM	Discrete Element Methods
ECS	Environmental Control System
HP NGV	High Pressure Nozzle Guide Vane
OPR	Overall Pressure Ratio
OSU	Ohio State University
SAS	Secondary Air System
TIT	Turbine Inlet Temperature

Roman Symbols

$\%t^*$	Percentage of time spent by a particle at a given orientation - see Chapter 4
$\bar{p}$	Vector of the particle's major axis, m
A	Cross sectional area of the OSU model cylinder, m ²
a	Contact patch radius, m - see Chapter 5 nomenclature
a_0	Equilibrium contact radius, m - see Chapter 5 nomenclature
A_{proj}	Particle projected area, m ²
C	Local mean particle concentration, kg m ⁻³
D_{Hell}	Hellinger distance $\frac{1}{\sqrt{2}} \sqrt{\sum_{x \in X} \left(\sqrt{P(x,y)} - \sqrt{Q(x,y)} \right)^2}$, m - Equation 17
D_h	Hydraulic diameter, m
D_p	Particle diameter, m
E	Elastic modulus, Pa
E_{act}	Collision activation energy (EBFOG model), J
E_{case}	Collision energy (EBFOG model), J
E_{crit}	Critical Young's modulus for plastic deformation, Pa - Equation 25
F_C	Elastic-adhesive pull-off force, N - see Chapter 5 nomenclature
F_n	Normal force at the contact patch, N - see Chapter 5 nomenclature
G	Shear modulus, Pa
k_t	Tangential stiffness of the contact patch, N m ⁻¹ - see Chapter 5 nomenclature
l	Length of the OSU model cylinder, m
L_{pass}	Passage length, m

L_{proj}	Particle projected length, m
m	Particle mass, kg
M_{ad}	Adhesion moment about particle centroid $4 F_C \xi \left(\frac{a}{a_0} \right)^{3/2}$, Nm - Equation 9
m_f	Fluid mass, kg
P	Particle perimeter, m
R	Particle radius, m
R_P	Particle radius of curvature following plastic deformation, m - see Chapter 5 nomenclature
Ra	Surface roughness level, μm
T_s	Particle softening temperature, K
u^*	Friction velocity, m s^{-1}
u_0	Reference flow velocity, m s^{-1}
V_n	Particle velocity normal to the surface, m s^{-1}
V_s	Particle-surface sliding velocity, m s^{-1}
V_t	Particle velocity tangential to the surface, m s^{-1}
V_f	Fluid velocity, m s^{-1}
W_A	Work of adhesion (van der Waals force), J
x_0	Squeeze-film thickness, m

Greek Symbols

$\bar{\Omega}$	Particle axis of rotation vector, m
δ_{equib}	Minimum separation distance between two surfaces in contact, m
δ_{gap}	Particle-surface separation distance, m
δ_n	Normal overlap between particle and surface, m
δ_t	Tangential displacement of the contact patch, m
η_n	Normal viscoelastic dissipation coefficient $\alpha \sqrt{m k_n}$, kg s^{-1} - Equation 10
γ	Surface free energy, J m^{-2}
μ_{crit}	Particle viscosity at the softening temperature T_s , Pa s
μ_f	Fluid dynamic viscosity, Pa s
μ_{T_P}	Particle viscosity at a temperature T_P , Pa s
ν_f	Fluid kinematic viscosity, $\text{m}^2 \text{s}^{-1}$
Ω	Particle angular velocity, rad s^{-1}
ω	Fluid angular velocity, rad s^{-1}
ρ_f	Fluid density, kg m^{-3}

ρ_p	Particle density, kg m^{-3}
σ_y	Yield stress, Pa
θ	Particle orientation angle, $^\circ$
θ_i	Particle impingement angle $\left[\tan^{-1} \left(\frac{V_{n0}}{V_{t0}} \right) \right]$, $^\circ$ - Equation 20
ξ	Adhesive rolling displacement, m
F_t	Tangential force at the contact patch, N

Non-Dimensional Groups

CoR_n	Normal coefficient of restitution $\frac{-V_{n3}}{V_{n0}}$ - Equation 18
CoR_t	Tangential coefficient of restitution $\frac{V_{t3}}{V_{t0}}$ - Equation 19
$\Delta\omega_y^+$	Normalised particle-fluid angular slip velocity about the y (spanwise) axis $(\Omega_y^+ - \omega_y^+)$
λ_T	Tabor parameter $\left(\frac{4R\gamma^2}{E^{*2}\delta_{\text{equib}}^3} \right)^{\frac{1}{3}}$ - Equation 7
ψ	Non-dimensional particle impingement angle $\frac{\kappa}{\mu} \tan(\theta_i)$ - Equation 5
τ_p^+	Non-dimensional particle relaxation time $\frac{C_c \rho_f \rho_p D_p^2 (u^*)^2}{18\mu_f}$ - Equation 15
Stk	Stokes number $\frac{\rho_p u_0 D_p^2}{18\mu_f l_0}$
Stk_c	Collision Stokes number $\frac{\rho_p V_{n0} D_p}{9\mu_f}$
V_d^+	Non-dimensional particle deposition velocity $\frac{1}{4} \frac{D_h}{L_{\text{pass}}} \frac{u_0}{u^*} \ln \left(\frac{C_{\text{in}}}{C_{\text{out}}} \right)$ - Equation 16
y^+	Dimensionless wall distance $\frac{u^* y}{\nu_f}$
AR	Particle aspect ratio $\frac{\pi L_{\text{proj}}^2}{4A_{\text{proj}}}$ - Equation 1
Re	Reynolds number $\frac{\rho_f u_0 l_0}{\mu_f}$
Sh	Particle shape factor $\frac{P^2}{4\pi A_{\text{proj}}}$ - Equation 2

Non-Dimensional Parameters

α	Non-dimensional material dependent viscoelasticity coefficient - Equation 10
$\alpha_{\text{frac}}, \beta_{\text{frac}}$	Material coefficients for minor and major fragmentation - see Figure 9
χ	Linear scaling of normal to tangential stiffness ratio $\left(\frac{7\kappa}{4} \right)$ - Equation 3
κ	Ratio of a particle's normal and tangential stiffness at impact $\frac{\frac{1-v_1}{G_1} + \frac{1-v_2}{G_2}}{\frac{1-v_1/2}{G_1} + \frac{1-v_2/2}{G_2}}$ - Equation 5
μ	Coulomb coefficient of friction
C_c	Cunningham correction factor
P_s	Particle sticking probability - Equation 21

v	Poisson's ratio
e_0	CoR _n where adhesion is the only energy dissipation mechanism
P	Prior deposition distribution (before the current sample)
Q	Posterior deposition distribution (before and including the current sample)

Subscripts

0	Far from the wall prior to the collision
1	At the point of collision
2	At the point of rebound
3	Far from the wall after rebound
el	Referring to elastic deformation
r	During particle rebound

Superscripts

*	Composite value between particle and surface
+	Normalised

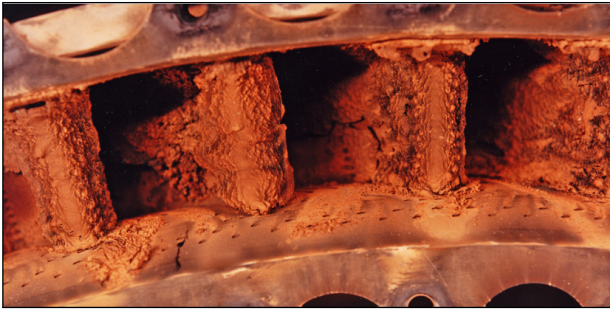


Figure 1: High pressure turbine vane deposition (Dunn, 2012).

Figure 2: Sand ingestion by a C-17 at takeoff (Walsh et al., 2006).

1 Introduction

The ingestion and deposition of atmospheric particulates are known to cause significant damage to gas turbine components. Coupled erosive, corrosive and geometry-altering depositive effects (Figure 1) risk the failure of hot gas path components and decrease operating surge margin. Second-order damage mechanisms arising from compressor surge and reduced cooling efficiency have further deleterious effects on efficiency, safety and operating costs throughout fleet service life. As the complete filtration of intake air is infeasible, the ability to accurately model deposition is essential to design particulate-tolerant hardware and predict the cost of ownership effects that arise from the ingestion of atmospheric contaminants.

Significant attention has been paid by the media and scientific literature to mass-deposition events that cause engine failure. Notably, British Airways Flight 009 and KLM Flight 867 which both suffered the loss of all four engines following flight through plumes of volcanic ash in 1982 and 1989 respectively, described by Clarkson et al., 2016. Repairs to the aircraft totalled tens of millions of dollars and prompted improved monitoring of volcanic dust clouds, pilot training and research into the effects particulate ingestion on gas turbines. Following the 2010 volcanic eruption of Eyjafjallajökull in Iceland, European airspace was largely closed to commercial traffic which disrupted the journeys of approximately 10.5 million passengers and cost the aviation industry USD\$1.7 billion of lost revenue (Budd et al., 2011). Military aircraft face systemic risks from mass-deposition events, often operating in regions with high atmospheric particulate concentrations and few established sites for takeoff and landing as shown by Figure 2: a C-17 ingesting sand through a ground vortex. Brun et al., 2012 documented an engine failure rate of up to 95 % on the US military's CH-47 helicopters during oper-

ation Iraqi Freedom while pilots resort to lifting-off before the recommended warm-up time to reduce particulate damage (Cardwell et al., 2010). In May 2015, a Bell-Boeing V-22 Osprey operated by the US Military suffered surge and engine failure following hover in brownout conditions, leading to a crash that killed two marines. A thirty second limit on hover in restricted visual conditions was subsequently imposed (Drew, 2019).

While the primary strategy to prevent mass-deposition events is avoidance, the same cannot be applied to the effects of low concentrations of particulates throughout the operating life of an engine. From 2016, sulphurisation of intermediate-pressure turbine (IPT) blades in Rolls-Royce Trent 1000 engines led to crack formation and unscheduled groundings of aircraft (Rolls Royce Plc, 2019). Sulphurisation occurred due to atmospheric contaminants in the secondary air system rather than the primary gas path, demonstrating that low-concentration exposure of particulates over a long period of time can have similarly deleterious effects as mass-deposition events. Deposit formation can also reduce the flow parameter of cooling passages, reducing cooling to hot gas path components and insulating surfaces from coolant, exacerbating particulate accumulation. Atmospheric particulate concentrations vary by orders of magnitude between regions and seasons (Kaspari et al., 2009) with differing compositions varying in their propensity to adhere (Dunn, 2012). The variability of particulate exposure therefore presents significant challenges to predicting engine maintenance requirements.

Modelling particulate deposition in computational fluid dynamics (CFD) software can be split into three main bodies of work: particulate transport, bounce stick modelling and deposit evolution and erosion. Particulate transport models are required to accurately predict the interaction between particulates and near-wall turbulent eddies to determine the location of particle-wall impacts. The bounce stick model is then used to predict whether the particle bounces, sticks or shatters and calculate the rebound trajectory, if appropriate. For simulations with significant deposition, a deposit evolution and erosion model is required to determine how successive layers of particulate matter interact with incoming particles. This may result in erosion or further accretion, coupled with the flow solution. The distinction between the deposit evolution and bounce stick models arises from the time scales considered. The bounce stick model considers only interactions comparable to the elastic response time of the collision, for example the London van der Waals force, while the evolution model works at much greater time scales, for example those related to heat transfer like sintering.

The present work describes the development of an experimentally-validated bounce stick model for use with CFD simulations of gas turbine secondary air system components. The research presented here comprises three main themes: simulations that explore relevant collision physics, to allow the specification of model requirements; development and validation of the model itself; and application of the model to gas turbine-relevant systems in CFD. Firstly, the sensitivity of rebound trajectories to particle rotation are explored in Chapter 3. This is complimented by Chapter 4, which determines the sensitivity of rebound to particle non-sphericity. In Chapter 5, the model is developed for single particle collisions, validated against existing experimental and numerical data from the literature. Finally, the implementation of the model in CFD is described in Chapter 6, with spatial distributions of deposition qualitatively validated by comparison to experimental data. Work presented in Appendix A provides a theoretical framework for predictions of particle rebound in rotating frames of reference, which is of particular relevance to particle deposition in rotating cavities.

The implementation of such a model in CFD will allow the design of deposition-tolerant hardware, for example through the inclusion of sacrificial components upstream of cooling passages. Predictions of fleet maintenance requirements may also be improved to reduce engine downtime and increase supply chain certainty. The efforts to develop this model are detailed through a combination of previously published research, accompanied by commentary, and standalone sections. Together, they describe the first experimentally-validated methodology, available in the open literature, for the predictions of spatially-resolved deposition in Lagrangian particle tracking simulations.

1.1 Publications Arising from Research

The thesis is presented in hybrid form, and the later chapters consist of a number of published and in-press papers with introductory sections placing them in the context of the overall research. A number of these papers are in draft form, but are extended versions of peer reviewed conference papers. A full list of publications from the research is provided below in Table 1:

Table 1: List of publications arising from the thesis.

Title	Reference	Thesis Chapter	Status
Collision-Induced Rotation and The Magnus Force on Particulates	Gaskell, J. G., Vadgama, N., McGilvray, M., Gillespie, D. R. H. Clarkson, R. J. (2020). "Collision-Induced Rotation and the Magnus Force on Particulates." Proceedings of the AIAA Aviation 2020 Forum. Virtual, Online. June 15-19, 2020. doi:10.2514/6.2020-2820	Chapter 3	Published
The Rebound of Non-Spherical Particles in Gas Turbine Components	Gaskell, J. G., McGilvray, M. Gillespie, D. R. H. (2021a). "The Rebound of Non-Spherical Particles in Gas Turbine Components." Proceedings of 14th European Conference on Turbomachinery Fluid Dynamics Thermodynamics. Virtual, Online. April 12-16, 2020. https://doi.org/10.29008/ETC2021-653	Chapter 4	Published
A Discrete Element Methods-based Model for Particulate Deposition and Rebound in Gas Turbines	Gaskell, J. G., McGilvray, M., Gillespie, D. R. H. (2021b). "A Discrete Element Methods-based Model for Particulate Deposition and Rebound in Gas Turbines." Proceedings of the ASME Turbo Expo 2021: Turbomachinery Technical Conference and Exposition. Volume 2B: Turbomachinery — Axial Flow Turbine Aerodynamics; Deposition, Erosion, Fouling, and Icing. Virtual, Online. June 7-11, 2021. ASME. https://doi.org/10.1115/GT2021-58477	Extended in Chapter 5	Published
Predicting and Validating Spatial Distributions of Particulate Deposition in Gas Turbine Components	Gaskell, J. G., Vadgama, N. Villain, Y.A., Beal, S., McGilvray, M., Gillespie, D. R. H. Littley, B. (2022a). "Predicting and Validating Spatial Distributions of Particulate Deposition in Gas Turbine Components." Proceedings of the ASME Turbo Expo 2022: Turbomachinery Technical Conference and Exposition. Volume 2B: Turbomachinery — Axial Flow Turbine Aerodynamics; Deposition, Erosion, Fouling, and Icing. Rotterdam. June 13-17, 2022. ASME.	Extended in Chapter 6	Published
Numerical Investigation of Particle Deposition in Double Wall Effusion Cooled Systems	Villain, F.Y.A., Vadgama, N., Gaskell, J.G., Ireland, P., McGilvray, M. Gillespie, D.R.H. (2022). "Numerical Investigation of Particle Deposition in Double Wall Effusion Cooled Systems." Proceedings of the ASME Turbo Expo 2022: Turbomachinery Technical Conference and Exposition. Volume 2B: Turbomachinery — Axial Flow Turbine Aerodynamics; Deposition, Erosion, Fouling, and Icing. Rotterdam. June 13-17, 2022. ASME.	-	Published
Modelling Particulate Deposition in Gas Turbines Part I: a Non-Spherical Bounce Stick Model	Gaskell, J. G., McGilvray, M., Gillespie, D. R. H. "Modelling Particulate Deposition in Gas Turbines Part I: a Non-Spherical Bounce Stick Model." ASME. J. Turbomach	Chapter 5	Submitted
Modelling Particulate Deposition in Gas Turbines Part II: Prediction and Validation of Deposition Distributions	Gaskell, J. G., Vadgama, N. Villain, Y.A., Beal, S., McGilvray, M., Gillespie, D. R. H. Littley, B. "Modelling Particulate Deposition in Gas Turbines Part II: Prediction and Validation of Deposition Distributions." ASME. J. Turbomach	Chapter 6	Submitted
Particle Bounce Stick Behaviour in the Rotating Frame of Reference	Gaskell, J. G., McGilvray, M., Gillespie, D. R. H. Irving, J. "Particle Bounce-Stick Behaviour in the Rotating Frame of Reference." ASME. J. Turbomach	Appendix A	Submitted

2 Literature Review

2.1 The Effects of Particulate Deposition

As discussed in Chapter 1, the ingestion of atmospheric particulates presents a significant hazard to jet aircraft. What concentrations of atmospheric particulates, particularly volcanic ash, are safe to fly through is subject to uncertainty in the open literature. Current ‘safe-to-fly’ limits are based on prior aircraft volcanic ash encounters, relating back casts of atmospheric volcanic ash concentrations to observed damage. In response to the 2010 eruption of Eyjafjallajökull in Iceland, Rolls-Royce proposed a safe flight limit of 2 mg m^{-3} (Clarkson et al., 2016). A preliminary sketch of an updated ‘safe-to-fly’ chart is shown in Figure 3 which also includes contours of long-term damage, based on historical service records of engines operated in particulate-laden environments. The chart in Figure 3 differs from the original 2010 ‘safe-to-fly’ chart as it also considers the duration of exposure. This modification is based on the assumption that engine damage is a function of the total mass of particulates ingested in-flight. While there are numerous mechanisms by which particulates may cause long-term engine damage, the proximate cause of flameout is accumulation of particulate matter on the high pressure nozzle guide vanes (HP NGV). Dunn, 2012 presents a comprehensive overview of damage mechanisms resulting from particulate matter, based on engine ingestion tests. The eight first-order damage mechanisms are:

- Deposition of foreign material in the hot gas path;
- Erosion of the compressor and turbine aerofoils;
- Cooling hole/passage blockage of the high-pressure turbine;
- Deterioration of the engine control system;
- Compressor aerofoil damage as a result of repeated engine surging;
- Oil/fuel system contamination;
- Ingestion by humans of very small particles passing through the Environmental Control System (ECS);
- Potential damage to electronic parts cooled by the ECS air.

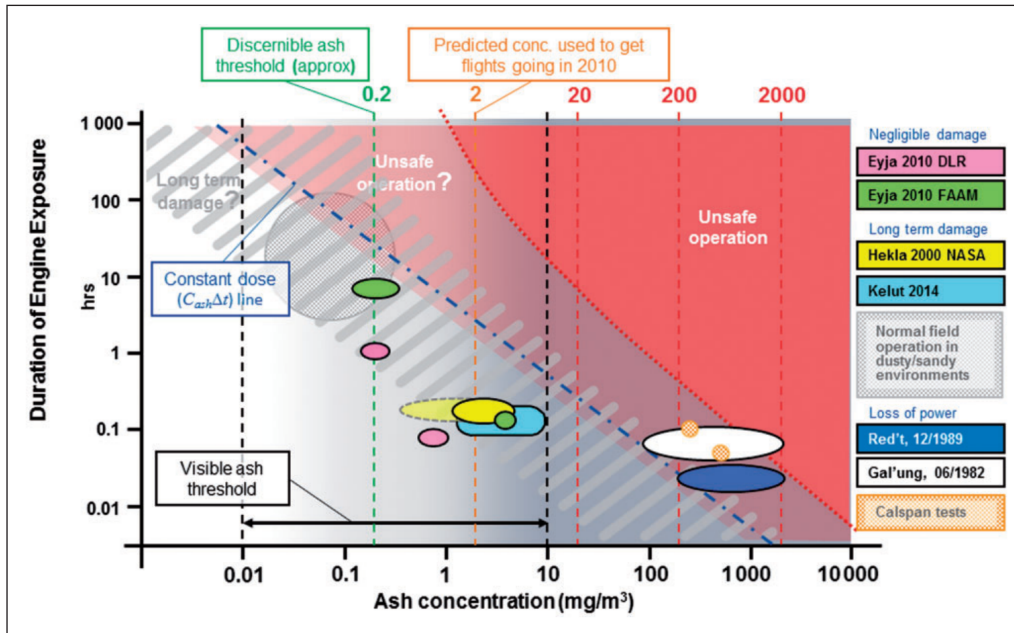
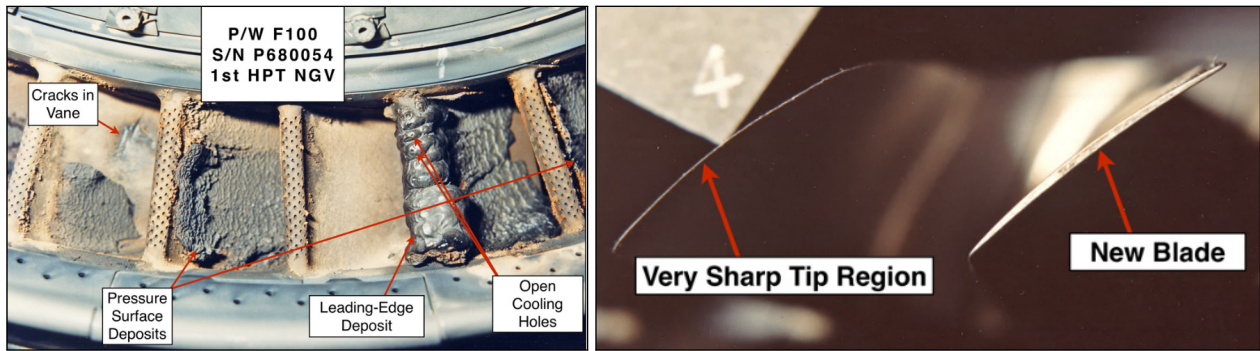


Figure 3: Duration of exposure vs. volcanic ash concentration with damage contours (Clarkson et al., 2016).

Dunn examined the performance of six engines, half with low turbine inlet temperatures (TIT) and half with TIT sufficient to cause significant deposition on hot-section components. In these high-TIT engines, surge was principally caused by a reduction in HP NGV throat width (Figures 1 and 4a) with additional losses due to compressor and turbine aerofoil erosion. At lower TIT, the primary damage mechanism and cause of surge was erosion (Figure 4b) and associated deformation of the aerofoils, for example thinned trailing edges bending away from the pressure surface. The greater overall pressure ratio (OPR) of higher TIT engines also exacerbates particulate deposition damage: increasing fluid density through the compressor raises the effective particle-volume fraction.

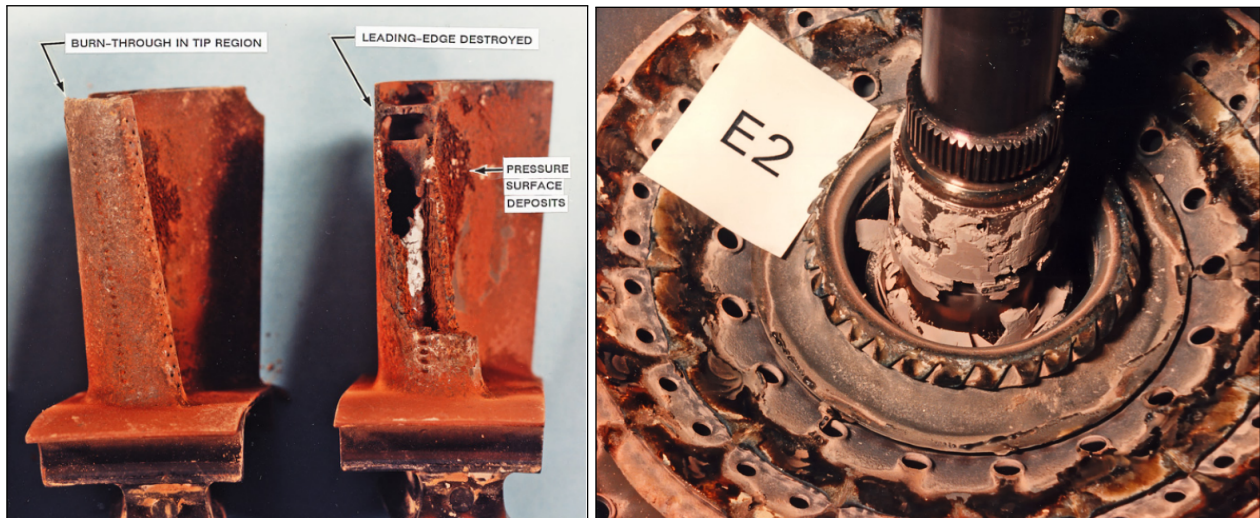
Attempts to relight engines following flameout were also hindered by fuel nozzle carbon deposits, caused by excessively rich combustion (Dunn, 2012). Post-deposition tests showed that the nozzles were still delivering sufficient fuel, but blocked swirl vanes were unable to provide sufficient atomisation. A contributory factor to surge and potential source of long-term damage to the engines is shown by the HP turbine blades in Figure 5a. Cooling passages and an upstream filter had become blocked, reducing coolant mass flow and contributing to the destruction of the blade tips and leading edges. At approximately $3.5\text{ }\mu\text{m}$ in diameter, the average particle entering the HP turbine cooling system was small enough to pass through the filter and block film cooling holes, exacerbating the decreased



(a) HP NGV deposition - note some deposition was removed for clarity.

(b) Fourth stage compressor erosion in comparison to a new blade.

Figure 4: Pratt & Whitney F100 engine damage from particulate ingestion (Dunn, 2012).



(a) HP turbine blades showing burn-through.

(b) Secondary air cavity deposition.

Figure 5: YF112 engine secondary air system deposition (Dunn, 2012).

coolant flow. Further evidence of secondary air system deposition is seen in Figure 5b that is likely related to the HP turbine damage. Dunn notes the significant quantity of a ‘talcum powder-like’ material that had circumvented the various seals and filters designed to prevent its accumulation. It is unclear whether deposits in the secondary air system will shed in a similar manner to those in the hot gas path on engine shut down, but it is clear that particulate matter can and does accumulate there in a manner that severely impedes safe flight.

More detailed experiments to characterise the blocking of cooling passages were performed by Walsh et al., 2006. Various test dusts were passed through a coupon, representative of a film cooling plate, at different temperatures and pressure ratios. Flow parameter reductions of up to 10% were ob-

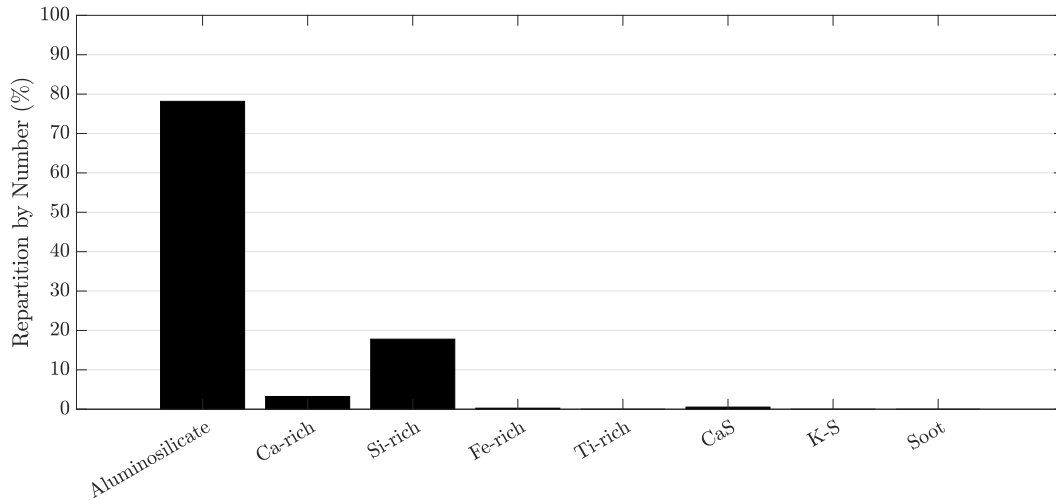


Figure 6: Mean elemental composition of super-micron atmospheric particulates from Chou et al., 2008.

served, with the magnitude of the reduction inversely related to the pressure ratio. This is likely due to lower velocity of the fluid and particle-wall collisions at low pressure ratios, discussed further in Chapter 2.3. This is supported by the increased relative deposition with greater flow areas, with a constant mass flow. Walsh et al. also observed the vicious circle of deposition: deposits insulate the surface from coolant, increasing metal temperature and further increasing deposition. Indeed, flow parameter reduction was a strong and non-linear function of metal temperature, increasing dramatically above the particulate softening temperature at approximately 1200 °C. This corresponds to results elsewhere in literature (Crosby et al., 2007). Cardwell et al., 2010 also simulated the passage of ingested particulates through a double-walled film cooling coupon. In ambient conditions, particle breakup on the upstream surface of the film cooling plate prevented the blockage of cooling holes. At engine-representative temperatures, this impingement led to deposition. Increased overlap between film cooling and impingement cooling holes therefore led to higher blockage of the film cooling holes.

2.2 Particle Properties

Chou et al., 2008 collected and analysed atmospheric dust samples from between 600-1500 m in altitude, representative of takeoff and landing conditions. Samples were collected over Niger, with Africa's 670 Mt annual emissions making it the world's largest source of mineral dust. Particulate concentrations reached a maximum of 1.2 mg m^{-3} , 60 % of the maximum concentration of volcanic ash permitted

by the ‘Safe-to-Fly’ chart in Figure 3. Collected particles above $0.4\mu\text{m}$ in diameter were primarily aluminosilicates: either illites, kaolinites or feldspars. Silicon-rich particles were also observed, mostly crystalline quartz. Similar studies of Saharan dust collected over Tenerife and Puerto Rico by Kandler et al., 2007 and Reid, 2003 respectively agree that aluminosilicates comprise the largest component of atmospheric dust at around 65 % by mass. While the elemental compositions are relatively homogeneous, the mechanical properties of different minerals may vary significantly. As larger particles are either centrifuged into the bypass duct or fragmented upstream of compressor bleeds, the atmospheric particle size distribution may not be representative of that of the secondary air system. However, substantial numbers of particles were found with diameters below $5\mu\text{m}$ that may enter the secondary air system unimpeded.

However, it should be noted that interactions may occur between the different minerals that comprise the particle when at elevated temperatures. For example. Nied et al., 2022 found that quartz chemically reacted with gypsum and dolomite, forming wollastonite and diopside. Each of these minerals may have different material properties, which are required as an input to bounce stick models. Elms et al., 2021 similarly noted that deposits formed in-engine contained a variety of high-temperature phases. Hence, the particle material properties measured prior to ingestion may not accurately represent deposition in-engine, especially in the hot gas path.

SEM images of collected particles show that most are non-spherical. Two parameters are commonly used to characterise their shape, aspect ratio (AR) and shape factor (Sh) as proposed by Reid, 2003. Aspect ratio refers to the approximate ratio of the length to width of the particle, Equation 1, assuming the particle can be approximated to a prolate spheroid. Shape factor refers to the effective roughness of the particle surface, Equation 2:

$$\text{AR} = \frac{\pi L_{\text{proj}}^2}{4A_{\text{proj}}} \quad (1)$$

$$\text{Sh} = \frac{P^2}{4\pi A_{\text{proj}}} \quad (2)$$

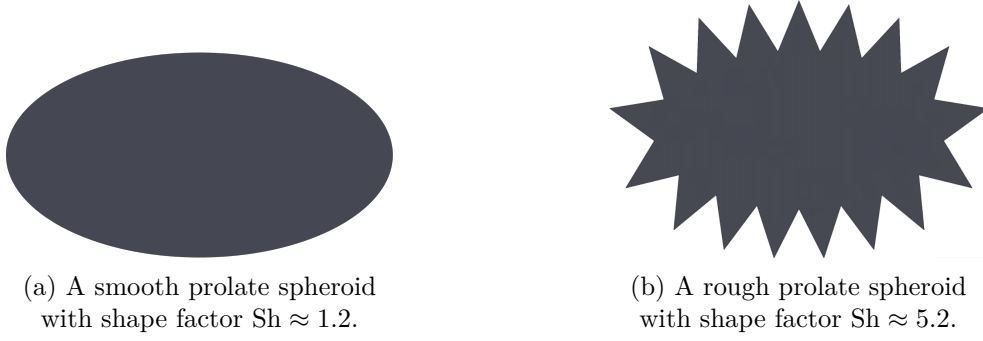


Figure 7: Comparison of shape factors for prolate spheroid-like particles of aspect ratio $AR \approx 1.9$.

where L_{proj} is the maximum projected length of the particle and A_{proj} is its projected area, while P is the particle perimeter. Figure 7 shows schematics of two prolate spheroid-like particles with the same aspect ratio of $AR \approx 1.9$ but different shape factors. Figure 7a shows a smooth particle with $Sh \approx 1.2$ while Figure 7b shows a rough particle with $Sh \approx 5.2$. Aspect ratio has little dependence on particle diameter, as shown by Figure 8a, where the median aspect ratio of sub- $10\ \mu\text{m}$ particles was 1.9. Similar results have been reported by (Chou et al., 2008) and Kandler et al., 2007 with $AR = 1.7$ and $AR = 1.6$ respectively. Shape factor varied significantly with particle diameter, where smaller particles had a more “jagged” shape. While the particles’ geometrical properties are well profiled in the literature, consistent mechanical properties are more challenging to acquire. For bounce stick modelling of volcanic ash, Bons et al., 2017 cites a Young’s Modulus (E) of 136 GPa, Poisson’s ratio (ν) of 0.2 and particle density (ρ_p) of $2320\ \text{kg m}^{-3}$. By contrast, Yu et al., 2016 cite values of E between 174 – 196 GPa for sand, depending on particle diameter. Meanwhile, nano-indentation experiments of Ottawa sand by Penumadu et al., 2009 estimated a Young’s Modulus of 105 GPa. Studies that measure all required properties of the right particulates are challenging to acquire. It is therefore necessary to develop models of deposition that are physics-based and independent of material properties as they vary with the origin of the particles and high-temperature chemical reactions. A material-independent model may also be validated with well-profiled engineering materials, where those of relevance to gas turbine deposition are not yet well profiled.

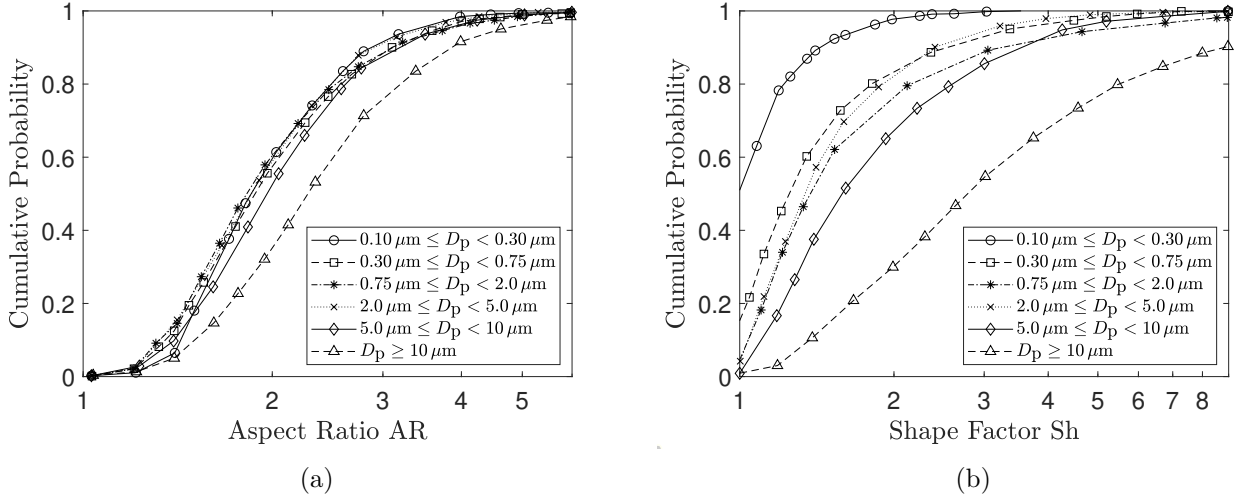


Figure 8: Airborne particulate morphology from Reid (2003)

2.3 Collision Physics

2.3.1 Particle Shatter & Fragmentation

Particle fracture and fragmentation causes uncertainty to bounce stick modelling, potentially introducing new discrete particles for tracking into the system. There are four key steps to modelling shatter in a gas turbine secondary air system:

1. Predicting the onset of fracture or fragmentation.
2. Determining the effect of attrition energy losses on the mean restitution of the particulate mass.
3. Determining how particle fragments behave post-collision, for example predicting the number and size of discrete particles ejected.
4. Modelling the trajectory of ejected fragments in a computationally efficient manner, as the number of particles tracked would theoretically grow exponentially with successive collisions.

Modelling fracture therefore first depends on determining when it occurs. Two approaches can be taken when modelling attrition: fracture mechanics and energetics. Fracture mechanics-based approaches model fracture and fragmentation by predicting crack initiation and growth. Papadopoulos, 1998 describes three distinct failure modes of particulates undergoing collisions with a flat surface: brittle, semi-brittle, and ductile. Brittle failure occurs with negligible plastic deformation near the contact patch, where cracks are initiated by preexisting flaws in the material. Predicting the onset

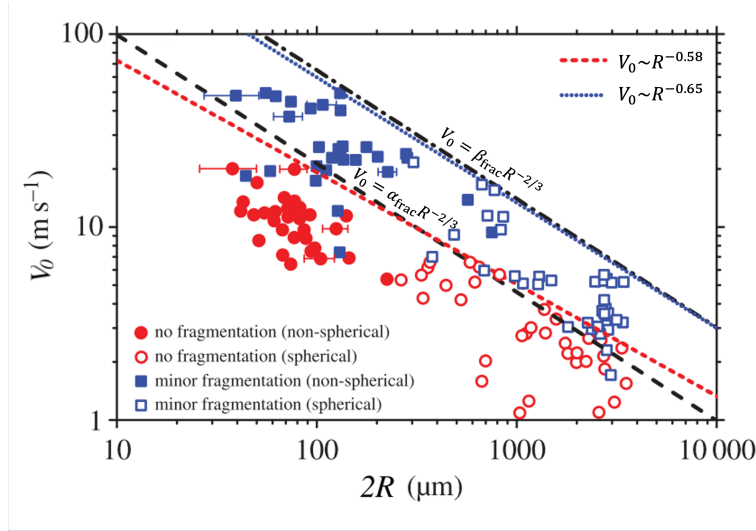


Figure 9: Boundaries of particle shatter against collision velocity and particle diameter from Hauk et al., 2015.

of brittle failure is therefore highly statistical, dependent as it is on the distribution of such flaws throughout the particle. Brittle failures are characterised by conical cracks that originate from the contact patch, reflecting the Hertzian stress profile during elastic deformation. Semi-brittle failure experiences a region of plastic deformation near the contact patch, which initiates cracks that propagate through the portion of the particle undergoing elastic deformation. With the region of plastic deformation acting as a stress concentrator, these cracks are typically large and cause the particle to separate into large pieces. Thornton et al., 1996 conducted numerical simulations of particle impact using a multi-element method, which also showed compression waves shattering the region of plastic deformation, ejecting a large number of small fragments. Ductile failure occurs when the region of plastic deformation reaches a particle boundary, where rupture occurs due to extensive shear deformation. Most experimental and numerical simulations of particle shatter model wall-normal impacts, although it should be noted that a tangential component of velocity introduces an asymmetrical stress distribution within the particle that increases the likelihood of fracture.

The energetics-based approach to failure is based on the work of Griffith, 1921. The onset of fracture is governed by the amount of potential energy stored in the particle during compression compared to the fracture energy required to form new crack surfaces. Considering the region of deformation near the contact patch, the stored potential energy is a function of the cube of the contact radius

a , i.e. the volume of the area compressed. However, the fracture surface energy is related to the area of the crack surface, proportional to a^2 , leading to a fundamental scaling law that governs crack initiation. Therefore, the ratio of energies that determines the onset of attrition has the dimension of length, usually the diameter of the region of plastic deformation. This means small particles are less likely to shatter than large particles. Hauk et al., 2015 performed a theoretical and experimental analysis of the shatter of ice particles. They determined analytically that the collision velocity that initiates cracking $V_0 \propto R^{-2/3}$. Therefore, by fitting experimental data to a material coefficient α_{frac} , they were able to predict particle fragmentation for a range of particle diameters and velocities, shown in Figure 9. Taking experimental values of the coefficient α_{frac} for different materials from Lecoq et al., 2003, the velocities at which shatter would be initiated for particles of interest in the secondary air system could be calculated. Lecoq et al. recorded that $400\text{ }\mu\text{m}$ diameter NaCl particles suffered fragmentation at a minimum collision velocity of 11 m s^{-1} , while $109\text{ }\mu\text{m}$ sand particles fractured at 65 m s^{-1} . Extrapolating the trend $V_0 = \alpha_{\text{frac}} R^{-2/3}$ from Hauk et al., $10\text{ }\mu\text{m}$ particles of NaCl and sand would shatter at 129 m s^{-1} and 319 m s^{-1} . These values are higher than the 100 m s^{-1} flow velocities that are typical of the secondary air system and represent ambient conditions. It is likely that the elevated temperatures would cause the particles to soften and increase the threshold velocity at which attrition initiates. Therefore, it is reasonable to assume that particles present in the secondary air system will not shatter.

2.3.2 Particle Dynamics

Accurate modelling of the contact patch shear is essential to predict frictional forces that determine the tangential rebound of the particle and its angular velocity post-impact. As described by Maw et al., 1976, at low impingement angles (where the particle glances the surface), the particle will slide throughout its contact with the wall (herein referred to as gross slip). This is due to a wall-normal impulse that is insufficient to reduce the particle-wall slip velocity to zero and induce rigid body rolling (herein referred to as gross roll). As the impingement angle is increased, the particle rolls for greater proportions of the total contact time. Maw describes this process using two non-dimensional parameters:

$$\chi = \frac{7\kappa}{4} \quad (3)$$

$$\psi = \frac{\kappa}{\mu} \tan(\theta_i) \quad (4)$$

Where μ is the Coulomb friction coefficient, ψ is the non-dimensional impact angle and χ is a function of κ , the ratio of the particle's normal and tangential contact stiffnesses at impact. A model of κ for two dissimilar materials as proposed by Johnson, 1985 is used:

$$\kappa = \frac{\frac{1-v_1}{G_1} + \frac{1-v_2}{G_2}}{\frac{1-v_1/2}{G_1} + \frac{1-v_2/2}{G_2}} \quad (5)$$

Using the above parameters, Maw describes three patterns of behaviour for the collision of an elastic sphere and a half space:

- **Sliding regime:** $\psi > 4\chi - 1$

The contact patch is in gross slip throughout the collision.

- **Intermediate regime:** $1 < \psi < 4\chi - 1$

Contact starts with gross slip but rolls during the collision. The point at which gross roll occurs gets earlier with more normal contact. After rolling, the contact patch reverts to gross slip before rebounding.

- **Sticking regime:** $\psi \leq 1$

The particle initially rolls, however after the midpoint of contact is passed and the particle starts to rebound gross slip is established.

Maw's model predicts the trend of frictional force acting on the contact patch, influencing the particle spin post-impact: friction with the surface induces a moment about its centre of mass and hence converts linear kinetic energy to rotational kinetic energy. The model is able to predict this transition by splitting the contact area into concentric annuli, each of which is treated separately when calculating tangential traction. This is necessary during an elastic collision as Hertzian theory assumes a parabolic normal pressure distribution at the contact patch. However, as explained in section 2.3.5, when perfectly plastic deformation occurs the pressure distribution at the contact patch plateaus. Therefore, Maw's model is only valid where the plastic strain induced by impact is small. Based on the same theory (Mindlin et al., 1953), Cundall et al., 1980 proposed an alternative method that treats the

contact patch as a mass-spring system. Shown by Equation 6, the contact patch is treated as a linear elastic spring - often including a damper - with extension δ_t , where the maximum elongation is limited by Coulomb friction.

$$F_t = -\min(|k_t \delta_t|, |\mu F_n|) \cdot \text{sign}(\delta_t) \quad (6)$$

As described by Kruggel-Emden et al., 2008, the model by Cundall et al. can be combined with a viscoelastic damping term, leading to five distinct tangential collision modes that alternate between gross slip and gross stick of the contact patch during a single collision. Kruggel-Emden et al. also note that where plastic deformation of the contact patch is significant, the tangential spring may no longer be constrained by the Coulomb condition. The addition of a damping term increases the accuracy of tangential rebound predictions when compared to experimental data.

When the particle is rolling with zero slip between the particle and substrate, particle angular velocity Ω is proportional to the inverse of its radius R^{-1} . As its angular kinetic energy is proportional to Ω^2 and R^5 , through the moment of inertia of a sphere, when rolling with a velocity V_t its rotational kinetic energy is proportional to R^3 . As incoming particle kinetic energy also scales with R^3 , the conversion of tangential kinetic energy to rotational kinetic energy will be significant at all scales. Friction will also cause a reduction in rebound velocities when the particle is sliding, which can be approximated using the normal force between the particle and surface, and the Coulomb friction coefficient μ .

2.3.3 Van der Waals Adhesive Forces

The London-van der Waals force is a weak inter-molecular interaction that is usually attractive. It has been shown by previous particulate modelling to become important to bounce stick behaviour for micron-scale particles (Bons et al., 2017; Brach et al., 1992; Wall et al., 1990; Crosby et al., 2008) and is the primary mechanism by which small particles will stick. There are four primary models of adhesion which are applicable for different values of the Tabor parameter (λ_T) as shown in Figure 10:

$$\lambda_T \equiv \left(\frac{4R\gamma^2}{E^* \delta_{\text{equib}}^3} \right)^{\frac{1}{3}} \quad (7)$$

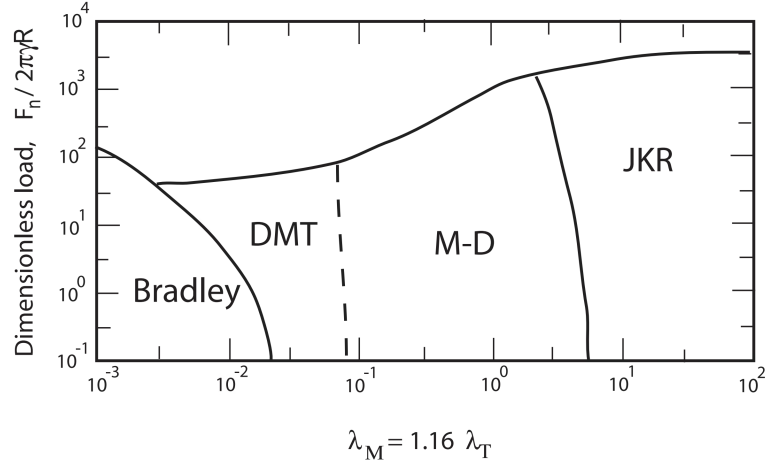


Figure 10: Different regimes of adhesive contact based on the Tabor parameter λ_T from Marshall et al., 2014

where δ_{equib} is the minimum separation between the two surfaces in contact. The Tabor parameter describes the relationship between the attractive adhesive force between the particle and surface, and the elastic compliance of the particle. Qualitatively, low values of the Tabor parameter describe small, rigid particles where adhesive forces are not sufficient to deform the contact patch. Large, soft spheres with high values of the Tabor parameter are more likely to deform due to adhesive forces and hence will generally have larger contact areas than described by Hertzian theory alone. The Bradley model is generally only applicable for very small, hard particles at the nanoscale and hence is not currently used for particulates in gas turbines (Marshall et al., 2014). The Derjaguin approximation (DMT model) relates the attractive force between concentric radii of two spheres where the minimum separation distance between the two spheres is much less than the radii of the spheres themselves. It assumes Hertzian contact where the force may act outside the contact radius. More commonly used is JKR theory (Johnson et al., 1971), which is widely used in literature (Bons et al., 2017; Yu et al., 2019; Chen et al., 2015). It assumes that adhesive forces only act within the contact radius but that the contact patch deforms due to adhesion and hence will be larger than the equivalent Hertzian prediction. Therefore, contact will be maintained even when the particle experiences negative normal load, “necking” as it is pulled from the surface. In both the DMT and JKR models, contact with the surface will be broken when the normal force at the contact patch reaches $-F_C$:

$$F_C = K\pi R\gamma \quad (8)$$

where K is either $3/2$ or 2 for the JKR and DMT models respectively. The Maugis-Dugdale (MD) model describes a more general solution where the DMT and JKR approaches are limiting cases. Micrometer-scale particles tend to have $\lambda_T > 3$ while the Tabor parameter decreases slowly with particle radius, scaling with $R^{1/3}$ (Marshall et al., 2014). Based on a $6\mu\text{m}$ particle of Arizona Road Dust (ARD) impacting stainless steel at ambient conditions $\lambda_T \approx 5$, within the range in which JKR theory is valid. This assumes that δ_{equib} can be calculated through the Lennard-Jones potential (Marshall et al., 2014), from the van der Waals radius of Carbon (Wolfram Research, 2014). Therefore, the JKR model is likely the most appropriate for use in gas turbine relevant applications, particularly as high temperatures will increase compliance of the contact patch. As the approach is force based, it does not directly prescribe an energy loss due to adhesion. However as experimental data shows a reduction in CoR_n in the presence of adhesion (Wall et al., 1990) a mechanism for kinetic energy dissipation must exist. Johnson et al., 1971 describe a “Work of Adhesion” term that accounts for adhesion hysteresis: the difference in energy taken to break an adhesive contact versus the lesser energy released when those surfaces are initially brought together. Ultimately, this is the source of energy loss due to adhesion. However, the dissipation pathway is not straightforward as the particle’s kinetic energy (resulting from normal velocity) is first transferred to elastic potential energy while the particle rebounds and “necks” due to adhesion. It is this stored elastic energy that allows the contact to be broken with associated viscoelastic losses due to the high strain rate (Chen et al., 2015).

During oblique impacts of small adhesive particles, adhesion may also affect tangential motion. The angular velocity acquired by the particle throughout the impact will be opposed by rolling friction. Without adhesion, rolling friction results from inelastic deformation, microslip at the interface and surface irregularities (Dominik et al., 1995). Viscoelastic losses are likely also significant. However adhesion plays an increasingly important role as particle radii decrease with kinetic energy scaling with R^3 and the contact area, hence work of adhesion, scaling with R^2 . During adhesive rolling, new contact between the substrate and particle surface is made continuously at the front of the contact area, while contact is continuously broken at the rear (Zhang et al., 2015). Due to adhesion hysteresis, this results in a loss of tangential kinetic energy. Dominik et al., 1995 developed a model of adhesive rolling friction based on the JKR model. When an angular displacement is first induced about the centroid of a spherical particle adhered to a flat surface, the contact patch remains stuck. This causes a horizontal displacement between the centre of the contact patch and the centroid of the particle, the

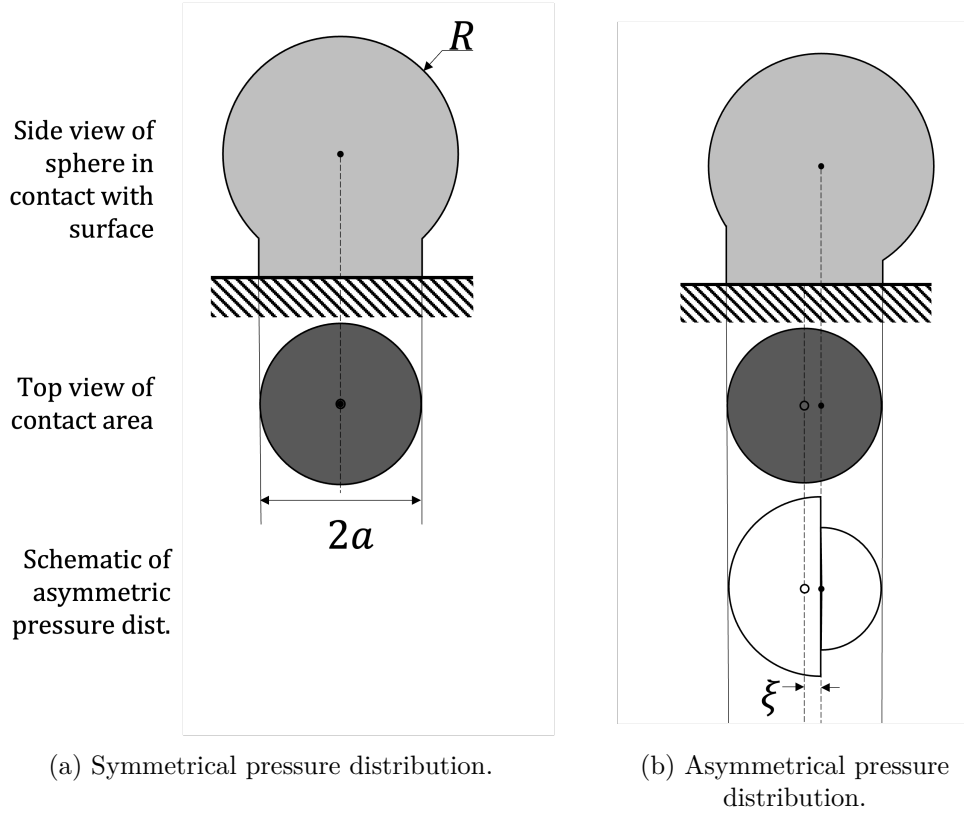


Figure 11: The onset of particle rolling in the presence of adhesion, from Dominik et al., 1995.

rolling displacement ξ , as shown in Figure 11. Once ξ reaches a critical value, ξ_{crit} , contact is broken at the rear of the contact patch and the contact patch as a whole begins to move at the same tangential velocity as the particle centroid, remaining ξ_{crit} behind the centroid. As can be seen in Figure 11, this is modelled as a discontinuous asymmetrical pressure distribution. The torque associated with adhesive rolling is expressed as:

$$M_{\text{ad}} = 4 F_C \xi \left(\frac{a}{a_0} \right)^{3/2} \quad (9)$$

where a is the contact radius and a_0 is the equilibrium contact radius, the radius at zero normal load.

In addition to adhesive effects, Wall et al., 1990 also studied the effects of electrostatic attraction of particulates to a surface. Micron-scale ammonium fluorescein spheres were fired at coupons of different materials, notably mica which normally held sufficient charge to attract a $5 \mu\text{m}$ diameter glass fibre

sphere held near the surface. Rebound was measured with and without exposure to a 500 μCi Po-210 source placed 5 mm from the coupon. A negligible difference in CoR_n was observed, indicating that the influence of electrostatics is small compared to van der Waals adhesion.

2.3.4 Viscoelasticity

Marshall, 2018 presents a sensitivity analysis of micron-scale adhesive particle rebound to different damping mechanisms. These include plastic deformation, squeeze film damping and viscoelastic deformation of the particle solid phase. As plastic deformation is generally treated as independent of strain rate, it is discussed separately in Chapter 2.3.5. However, the velocity dependence of squeeze film and solid phase viscoelastic damping would allow a physical explanation for other velocity-related terms used to fit collision models to experimental data (Bons et al., 2017; Chen et al., 2015). The normal dissipative force associated with solid phase viscoelastic damping F_{nd} is calculated as the product of the normal velocity of deformation V_n and a dissipation coefficient η_n . Through simple dynamics, the dissipation coefficient is a function of the particle mass m , some stiffness coefficient k_n and a material coefficient α :

$$\eta_n(t) = \alpha \sqrt{m k_n(t)} \quad (10)$$

where k_n is the product of the composite elastic modulus E^* and contact radius a . The dependence on contact radius makes the normal dissipative force time-variant during the collision. Marshall, 2009 showed that where particle deformation was treated as a simple mass-spring-damper system, the material coefficient α was the only factor affecting rebound (all other coefficients having been removed by scaling). As solid phase viscoelastic damping is the only dissipation mechanism in the simple system, by solving non-dimensional equations of motion for different values of α , a relationship between α and CoR_n could be determined. Marshall, 2009 presents a sixth-order polynomial fit between CoR_n and α , allowing an appropriate material coefficient to be fitted to collision data. The approach allows a physically-correct model of viscoelasticity with fitting to a single collision data point, however it does assume that work hardening will not significantly alter the stiffness of the particle in high-velocity impacts. Marshall, 2018 also presents a method to account for viscoelastic squeeze film damping. Squeeze film damping refers to viscous dissipation in the thin film fluid between the particle

and surface shortly before and after a collision occurs. The strength of the damping effect depends on the ratio between the particle stopping time and the fluid convective time scales, the collision Stokes number Stk_c :

$$\text{Stk}_c = \frac{2\rho_p V_{n0} R}{9\mu_f} \quad (11)$$

where V_{n0} is the particle wall-normal velocity far from the wall. By calculating the damping force as a function of the minimum separation distance and integrating, an equation that relates the velocity close to and far from the wall can be derived:

$$\frac{V_{n1}}{V_{n0}} = 1 + \frac{1}{\text{Stk}_c} \ln(\delta_{\text{gap}}/x_0) \quad (12)$$

where δ_{gap} is the separation distance, effectively surface roughness for real particulates, and x_0 is the squeeze-film thickness equal to $0.01R$ (Davis et al., 1986). Marshall showed that the combination of squeeze film damping and solid phase damping were both essential to allowing a match between models and experimental collision data, when combined with models of plastic deformation and adhesion.

2.3.5 Plastic Deformation

At large normal collision velocities, where adhesion is negligible, plastic deformation is the primary source of kinetic energy loss for normal collisions. At first contact with a flat plate, the pressure distribution of a sphere's contact patch will be parabolic according to Hertzian theory. As described by Johnson, 2004, through both the Tresca and von Mises criteria, peak stress will occur below the contact surface. For the axi-symmetric contact of solids of revolution, plastic deformation will occur when the maximum contact stress reaches $1.6\sigma_y$. The yield stress, σ_y , is taken to be the minimum from each of the bodies. Plastic deformation will cause the pressure distribution to flatten, reaching a maximum value of approximately $2.7\sigma_y$. This is shown by Figure 12 where FEA results are compared with Hertzian theory. Jackson et al., 2005 present a model for plastic deformation that is fitted to FEA results, finding that the exact limiting contact pressure varies with the geometry of the deformed contact and material, between $2.59\sigma_y$ and $2.80\sigma_y$. However, the material dependency presents challenges for a general, material-independent formulation.

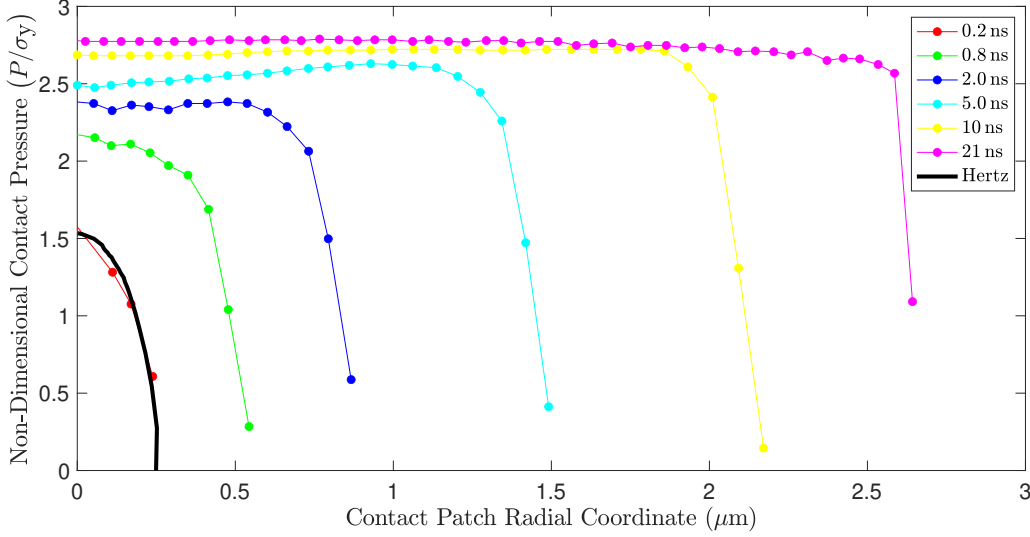


Figure 12: Evolution of the contact pressure distribution of a sphere and rigid surface during compression, showing flattening with increasing plastic deformation. Contact pressure P is normalised by yield stress σ_y . Figure from Wu et al., 2003.

Thornton et al., 1998 derived a normal rebound model for the elastic perfectly-plastic adhesive impact of spheres. The model describes three stages of impact: elastic compression, perfectly-plastic deformation and elastic-adhesive unloading. In Figure 13, elastic compression is shown between points one and two: the sphere behaves according to Hertzian theory as modified by Johnson et al., 1971 to account for adhesion. If yield does not occur, elastic JKR theory is used to describe the whole contact and will follow the curve described by $F_{n,el}$. If the maximum surface pressure reaches $1.6\sigma_y$, yielding occurs (point two) and the contact stiffness is fixed at a constant value with the particle deforming plastically until the point of maximum penetration, where $V_n(t) = 0$ at point three. A new effective radius of curvature, R_P , is then calculated to account for flattening of the contact patch due to plastic deformation. This new contact radius is substituted into the elastic JKR equations to describe rebound, denoted by subscript r from point three onward. The elastic potential energy stored during compression is converted back into kinetic energy, with the particle rebounding between points three and five. Contact is broken according to JKR at point five, with the contact patch “peeling” after point four. Thornton and Ning’s model is crucial to understanding how adhesive contacts are affected by plastic deformation and is the most comprehensive model of coupled adhesive-plastic behaviour currently available in the literature (Thornton et al., 2017) and avoids the non-physical behaviour of

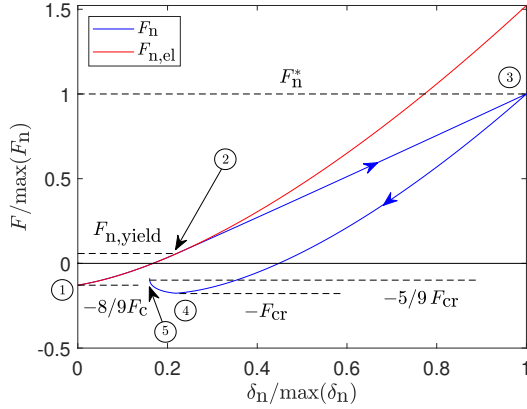


Figure 13: Normalised force-displacement plot of a highly plastic adhesive impact of a sphere vs. a flat plate. Actual normal contact force F_n and equivalent elastic normal force $F_{n,el}$ are shown. From Gaskell et al., 2021b

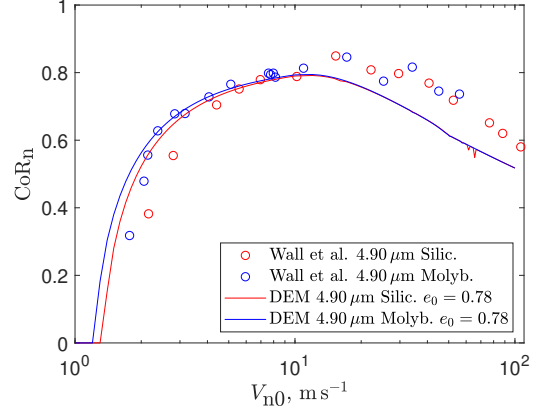


Figure 14: Normal coefficient of restitution for impacts with varying γ . Adhesive losses at low normal impact velocities and plastic losses at high normal impact velocities. From Gaskell et al., 2021b

simpler, piece-wise linear models like those described by Luding, 2005. Thornton and Ning's model prescribes a limiting contact pressure of $2.4\sigma_y$, based on the truncation of the Hertzian parabolic pressure distribution.

Plastic deformation reduces the CoR_n of impacting particles where the maximum normal contact force is sufficient to initiate yield. This occurs above a critical yield velocity, above which it can be shown analytically that CoR_n scales with $V_n^{-0.25}$ (Thornton et al., 2017). This is shown clearly by simulations in Figure 14 and corroborated by the experimental results described in Wall et al., 1990. With differing values of γ , adhesive losses are limited to low normal impact velocities while losses at high velocities are dominated by plastic deformation.

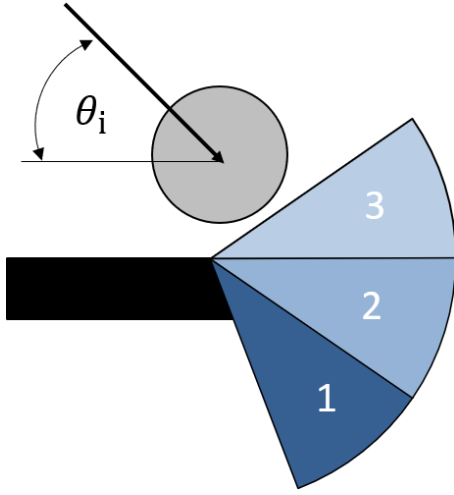
2.3.6 Surface Roughness

Surface roughness has been shown experimentally to alter the rate, location and quantity of deposition in gas turbine representative conditions (Wammack et al., 2008). Deposits roughen aerodynamic surfaces which increases the rate of heat transfer and surface friction. Wammack et al. used an accelerated deposition facility to study how a deposit evolves at a Mach number of 0.31 and freestream temperature of 1150°C . Three coupons were used: (1) polished metal with roughness level $Ra = 0.1\mu\text{m}$; (2) polished thermal barrier coating with $Ra = 0.6\mu\text{m}$; and (3) unpolished bondcoat where $Ra = 16\mu\text{m}$. Successive deposition tests caused the coupons to alternate between rough and smooth as peaks were

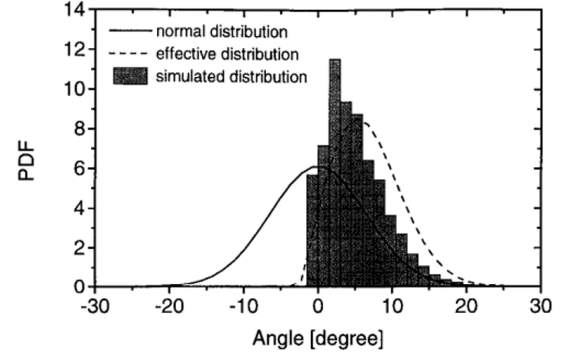
formed by deposits and the valleys between them subsequently filled. Incoming particles are also more likely to collide with existing deposits as the mass deposited increases, altering the particle-surface interaction. A vicious circle develops where deposits insulate hot gas path components from coolant, increasing surface temperature and the rate of deposition. However, deposit evolution and growth is a complex topic that must include second-order effects like erosion (Bowen et al., 2021).

If the scale of the roughness structures are much greater than the particle diameter then surface roughness will affect the effective angle of incidence between the particle and surface. Sampling the height of the surface at different points will allow a statistical distribution of surface roughness angles to be determined. This distribution may reasonably be assumed to have a mean of zero, with positive and negative angles cancelling each other out. However, as shown by Sommerfeld et al., 1999 the surface roughness cannot always be approximated as a symmetrical normal distribution: the so-called ‘shadow effect’ will increase the likelihood of a particle impacting a roughness structure with a positive gradient. Figure 15a shows how, for small impingement angles, a particle may avoid a section of the roughness structure that has a negative inclination angle. Therefore, it would be more likely to collide with a roughness structure at a positive inclination angle. This is demonstrated in Figures 15b, 15c and 15d which show how the inclination of the surface roughness is effectively shifted for small impingement angles. This will increase the rate of transfer between tangential and normal momentum as more particles collide with an inclined surface, effectively increasing CoR_n while decreasing CoR_t . In the first order, this will likely decrease the rate of deposition as the particle experiences higher effective normal impact velocities. The effective angle of incidence is simply the sum of the roughness angle and the actual incidence angle. With reference to Figure 15a, three scenarios are possible:

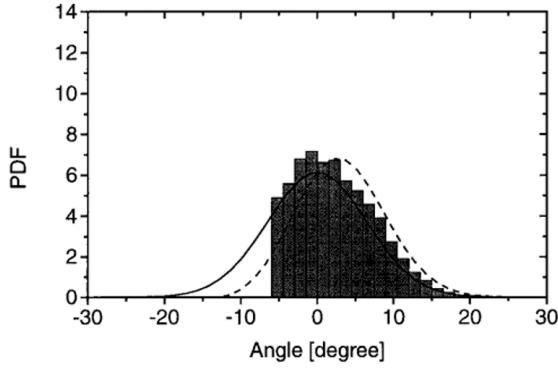
1. The particle cannot collide with a roughness structure where the negative inclination is greater than θ_i ;
2. The probability of colliding with negative inclination angles is reduced with small values of θ_i ;
3. The probability of colliding with a wall with positive inclination is higher with increased θ_i .



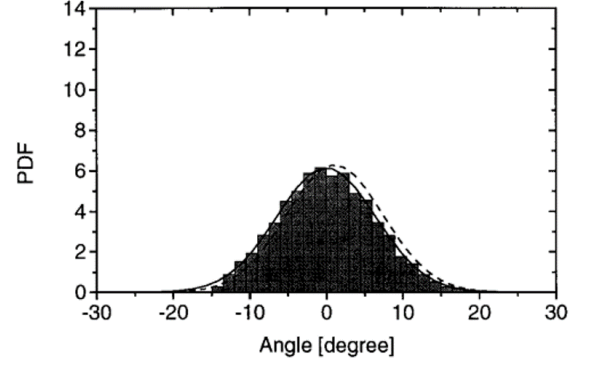
(a) Illustration of shadow effect for small impingement angles



(b) $\theta_i = 2.5^\circ$



(c) $\theta_i = 12.5^\circ$



(d) $\theta_i = 32.5^\circ$

Figure 15: The shift in roughness angle probability distribution for increasing incidence angles θ_i due to the shadow effect. Figures from Sommerfeld et al., 1999.

2.3.7 Temperature

Crosby et al., 2008 simulated ash deposition in a land-based gas turbine HP NGV at elevated gas temperatures, finding that capture efficiency increased from 0 % at 860 °C to 1.8 % at 1183 °C. Capture efficiency is defined as the mass flow rate of particulate that deposits divided by the mass flow rate of particulate that is added to the flow. In physics-based bounce stick models, increasing temperature is generally modelled by decreasing Young's modulus, for example by Bons et al., 2017. Higher temperatures therefore lead to greater deformation, a larger contact area and a greater adhesive pull-off force. This assumption holds where the particle boundary is continuous, below the temperature at which the contact patch will melt. This approach was demonstrated in CFD by Ai et al., 2012, where predicted capture efficiencies showed good agreement with experimental data. The trend of capture efficiency -

the ratio of injected particles that stuck - and sticking efficiency - the ratio of impacting particles that stuck - with temperature are shown in Figure 16. Figure 16a clearly demonstrates that decreasing size and increasing temperature causes particles to stick. However, Figure 16b shows that this is offset by the low Stokes number of small particles reducing the chance they will collide with a wall, meaning deposition is highest at intermediate particle sizes. In both cases, temperature significantly increased the amount of material deposited. The Stokes number Stk is the ratio of particle and fluid response times. Particles with a Stokes number much greater than one behave ballistically, while those with a value much less than one will follow the flow. Note that the Stokes numbers given in Figure 16 are approximate, assuming that the dynamic viscosity of air is constant at an average temperature of 1373 K. Stokes number is defined here as in Equation 13, with the relevant length and velocity scales, l_0 and u_0 defined by the length and outlet velocity of the impinging jet from Ai et al., 2012.

$$Stk = \frac{\rho_p u_0 D_p^2}{18\mu_f l_0} \quad (13)$$

Temperatures in the secondary air systems are generally lower than those in the main gas path. Inlet air temperature near the hub will be comparable to the compressor outlet at approximately 850 K, increasing with proximity to the turbine blades and stators. However, conjugate heat transfer simulations of cooling geometries and rotor-stator cavities show that gas temperatures generally do not exceed the 1300 K softening temperatures of most ingested atmospheric particulates (Ho et al., 1996; Vadvadgi et al., 2010). Deposition is also sensitive to metal temperature, due to contact during collisions and radiative heating when near the wall (Cardwell et al., 2010). With effective cooling strategies blade metal temperatures generally still do not exceed particulate softening temperatures, peaking at approximately 1200 K in a spanwise average TIT of 1480 K (Alizadeh et al., 2014). Particulates in the secondary air system can therefore be treated as solids, avoiding methods that consider particle splashing. Indeed, dimensional analysis of particle impacts demonstrates that splashing generally requires temperatures that are approximately three times that of the softening point, above 3000 K (Suman et al., 2019).

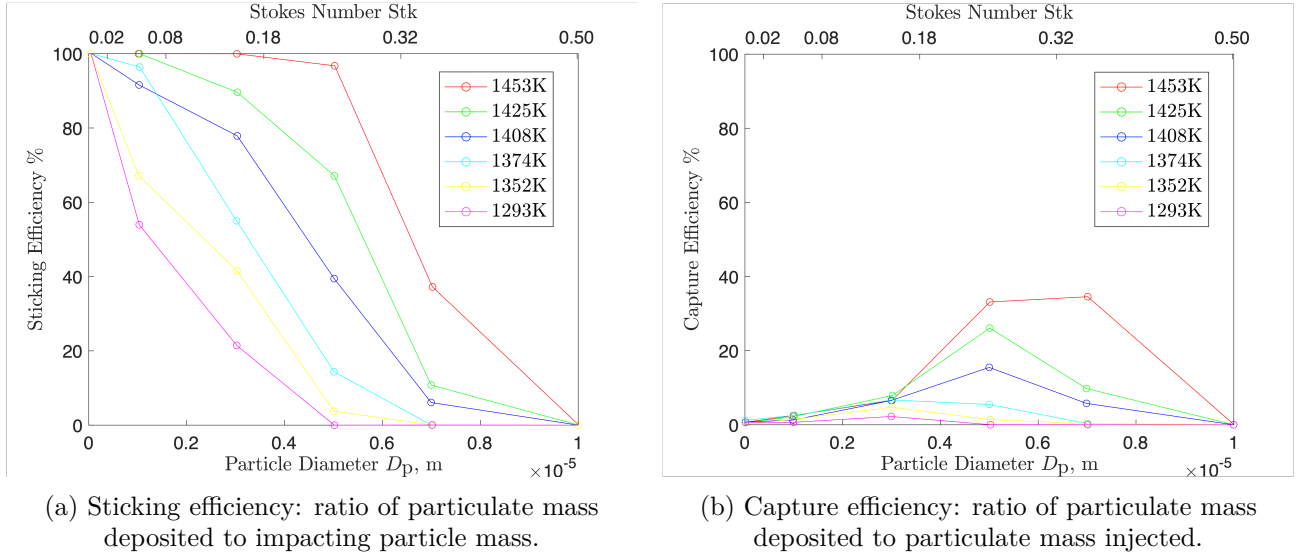


Figure 16: Variation of sticking and capture efficiencies with particle diameter, gas temperature, and Stokes number, predicted by CFD from Ai et al., 2012. Note that Stokes number is defined here in Equation 13.

2.4 Particle Tracking

Where a bounce stick model calculates the particle trajectory at rebound, or predicts sticking, particle tracking models are used to predict how the particle interacts with the flow. Hence, they determine the location and velocity at which a particle will impact the wall. Particle acceleration can be calculated by the summation of six terms, where the particle Reynolds number is much less than one (Cartwright et al., 2010):

$$\begin{aligned}
 \frac{dmV}{dt} = & -6\pi R\mu_f(V - V_f) + (m - m_f)g - m_f \frac{DV}{Dt} \\
 & - \frac{1}{2}m_f \left(\frac{dV}{dt} - \frac{DV_f}{Dt} \right) - 3\pi R^2\mu_f \int_0^t \left(\frac{dV_p}{d\tau} - \frac{dV_f}{d\tau} \right) \frac{1}{\sqrt{\pi\nu(t-\tau)}} d\tau \\
 & + m_f C_L (V_f - V) \times \omega + 3.22\mu_f R (V_f - V) \sqrt{Re} \quad (14)
 \end{aligned}$$

These terms represent drag, gravity and buoyancy, pressure gradient, added mass, Basset history, Magnus lift and Saffman lift. Saffman lift is the lift force due to fluid shear across the particle. Electrostatic forces may also influence particle motion, but are treated separately to forces that originate from the fluid. The drag force may be calculated using drag coefficient calculations where the particle

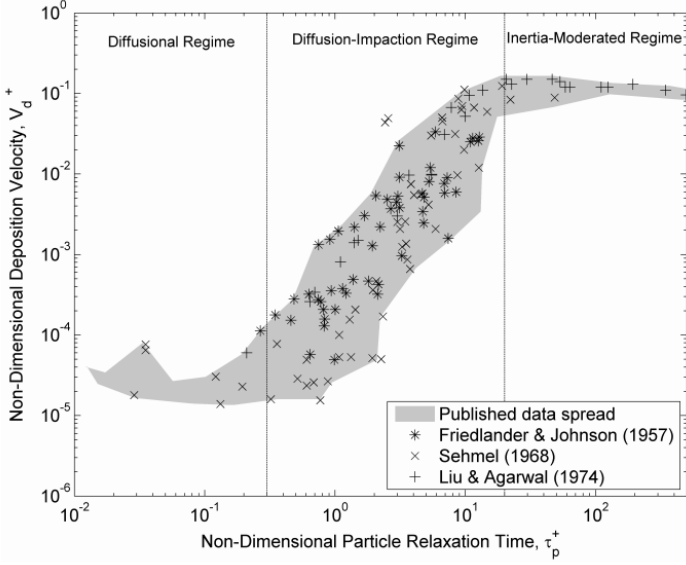


Figure 17: Particle deposition regimes from Forsyth et al., 2016

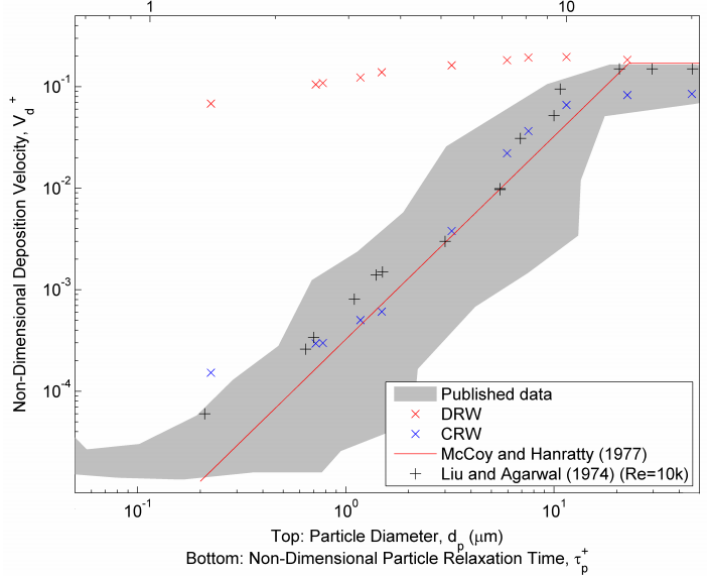


Figure 18: Comparison between the DRW and CRW from Forsyth et al., 2016

Reynolds number is greater than one. The forces that result from pressure gradient, added mass and buoyancy are of the order (ρ_f/ρ_p) , which are likely to be small even at the high pressure ratios achieved by modern propulsive gas turbines (Borello et al., 2016). Similarly, the Basset history force is of order $\sqrt{\rho_f/\rho_p}$. The Magnus force is often neglected in particle tracking in place of the Saffman force. It has been shown analytically that the Magnus force resulting from rotation due to fluid shear is always much less than the Saffman lift due to shear itself (Saffman, 1965; Zhou et al., 2015). However, this neglects other causes of particle rotation like collisions with a wall.

Particle motion is also affected by fluid temperature gradients: thermophoresis results from an unequal exchange of momentum between the particle and fluid molecules across its surface (Forsyth, 2017). The high temperature fluid imparts more energy to the particle, causing a force that acts down the temperature gradient. Where particles are present in the cooling flow of gas turbines, high metal temperatures will reduce deposition. However, the same effect in the hot gas path will increase the rate of deposition.

Turbophoresis is the phenomenon that causes particles to migrate from regions of high turbulence to low turbulence (Johnson et al., 2020). The difference in turbulent dispersion rates between these regions causes particles to accumulate preferentially in the viscous sublayer and buffer region, due to the sharp gradients of turbulence intensity near the wall. Particle interaction with near-wall coherent structures like streamwise vortices, ejections and in-sweeps increase deposition, on average, however the process is necessarily stochastic. The rate of deposition is often expressed as the non-dimensional deposition velocity V_d^+ . Expressions for τ_p^+ and V_d^+ for a closed passage are given by Equations 15 and 16. Considering turbophoretic effects, three regimes of deposition exist: diffusional, diffusion-impaction and inertia-moderated (Vadgama, 2021). They are shown with reference to V_d^+ and τ_p^+ in Figure 17. Particle impaction in the diffusional regime is governed by Brownian motion, where V_d^+ is not affected by particle diameter (which is analogous to non-dimensional particle relaxation time in this case). In the diffusion-impaction regime, turbulent eddies impart energy to the particle which leads to a significant increase in V_d^+ with τ_p^+ . In the inertia-moderated regime, the increasing inertia of the particles relative to force imparted by eddies reduces the influence of turbulence on particle motion, hence decreasing the sensitivity of V_d^+ to τ_p^+ .

$$\tau_p^+ = \frac{C_c \rho_f \rho_p D_p^2 (u^*)^2}{18 \mu_f} \quad (15)$$

$$V_d^+ = \frac{1}{4} \frac{D_h}{L_{\text{pass}}} \frac{u_0}{u^*} \ln \left(\frac{C_{\text{in}}}{C_{\text{out}}} \right) \quad (16)$$

Where turbulence is modelled in CFD, the instantaneous fluctuating velocities experienced by the particle must be approximated to account for turbophoresis. Two models popularly used are the Discrete Random Walk (DRW) and the Continuous Random Walk (CRW). The DRW assumes that the velocity fluctuation experienced by a particle is constant over the length of an eddy, derived from a Gaussian probability distribution. The CRW models the unsteady velocity experienced by a particle during its interaction with a single eddy which eliminates the over prediction (shown by Figure 18) of the deposition velocity by the DRW (Forsyth, 2017; Vadgama, 2021; Forsyth et al., 2017). However, acquiring the necessary turbulent statistics to apply the CRW to RANS flow solutions is challenging, with many versions of the CRW relying on data from DNS solutions. This necessarily limits the CRW

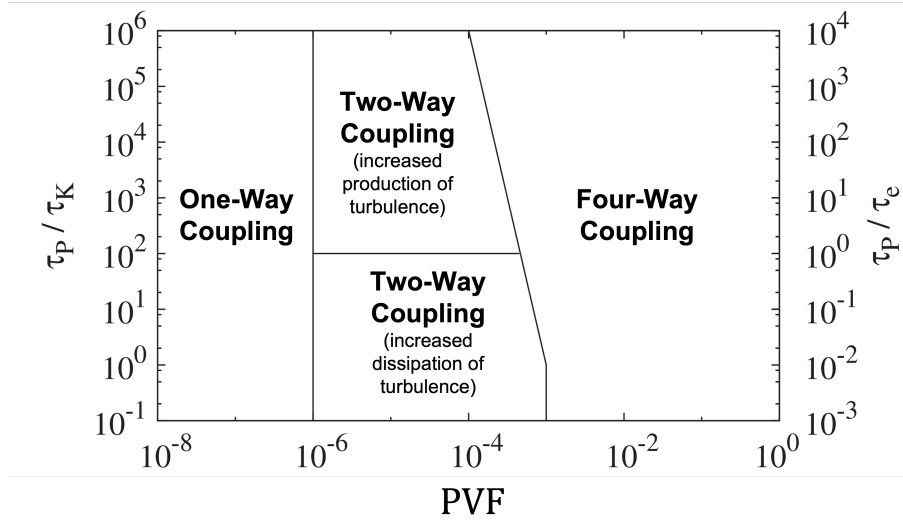


Figure 19: Classification of particle-fluid coupling regimes, from Greifzu et al., 2016. Note that τ_p is the particle timescale whilst τ_k and τ_e are the Kolmogorov and eddy timescales respectively.

to simple flows, however further developments using Reynolds Stress Models (RSM) now allow the CRW to be applied to more complex flow cases (Vadgama et al., 2020b).

Particulate tracking in CFD simulations relevant to gas turbines is usually Lagrangian (Vadgama, 2021; Forsyth, 2017), which is more appropriate for low particle-volume fractions (PVF) as described by Saidi et al., 2014. Three methods of coupling the discrete and fluid phases of the solution are possible: one-way coupling; two-way coupling; and four-way coupling. During one-way coupling, the particles are assumed to have no interactions with one another and no effect on the fluid solution. Two way coupling assumes that the PVF is sufficient for particles to influence turbulence in the flow. Finally, four-way coupling assumes that the particles interact with the flow and each other, at the highest values of PVF. The particle volume fraction is defined as the total volume occupied by the discrete phase of a solution compared to the fluid phase. Figure 19 shows the method of coupling required for increasing PVF. Assuming a worst-case flight scenario from Clarkson et al., 2016 where 2 mg m^{-3} of particulate is ingested and a high pressure ratio civil turbofan, the PVF remains at least two orders of magnitude below the limit at which two-way coupling is necessary, 10^{-6} (Vadgama, 2021).

With a time-invariant fluid solution, simple Lagrangian particle trajectories at constant injection points will be spatially deterministic. Introducing a stochastic model like the CRW necessitates multiple particle injections to ensure converged deposition profiles. As described by Vadgama et al., 2020a, the convergence of integral deposition does not necessarily guarantee spatial convergence. Graham et al., 2002 found that the uncertainty in spatial distributions was only a function of the total number of particles injected. They proposed a method to quantify the uncertainty that involves first varying the number of particle injections N_s , with a nominal number of particles per injection, until convergence is achieved. They then increase the number of particles per injection N_p until the trend of the maximum standard deviation from all injections is proportional to $N_p^{-1/2}$. The local maximum sample standard deviation can then be used to determine how to obtain the required accuracy. Vadgama et al., 2020a proposes a simpler method that uses the Hellinger distance to determine spatial convergence:

$$D_{\text{Hell}}(P||Q) = \frac{1}{\sqrt{2}} \sqrt{\sum_{x \in X} \left(\sqrt{P(x,y)} - \sqrt{Q(x,y)} \right)^2}. \quad (17)$$

In Equation 17, P and Q refer to the prior and posterior deposition distributions respectively: the distribution before the current sample and including the current sample. The Hellinger distance is first calculated using increasing N_p with a single sample, then with increasing N_s and the N_p from the previous step. Normalising the distance by the integral deposition fraction allows a universal comparison of spatial convergence, Vadgama et al. setting a convergence threshold of 10 %.

2.5 Deposition Models

A number of deposition models currently exist in literature that vary in complexity, computational intensity and dependency on empirical data. Most existing models require significant parametric fitting where single particle collision data, collected experimentally, is used to modify material parameters. While this results in accurate predictions of rebound for specific use cases, the model will not necessarily be generalisable to novel material pairs, particle sizes, temperatures or shapes. Indeed, applying non-physical corrections to simulation input parameters may negatively impact other aspects of the model. For example modifying the process of plastic deformation may affect predictions of contact area and therefore van der Waals adhesion.

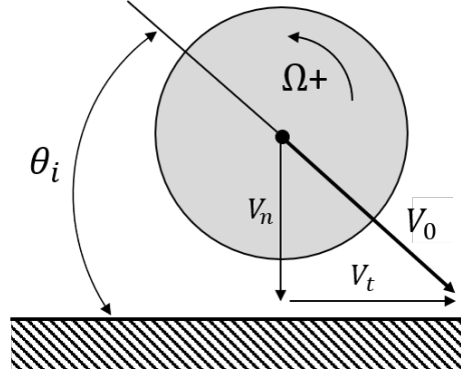


Figure 20: Particle sign convention.

The capabilities of existing models also vary, from those that calculate only a probability of sticking to some that predict rebound for components normal and tangential to the wall. Where a prolate spheroid impacts a smooth wall with a velocity vector in the same plane as its major axis, with no angular velocity about that axis, the impact is planar. The linear components of rebound can therefore be described using two parameters: the normal and tangential coefficients of restitution (CoR_n and CoR_t). The rotational component is described using a single angular velocity Ω about its centroid through the axis into the page in Figure 20. The coefficients of restitution are defined as the ratio of incoming and outbound velocity components far from the wall, Equations 18 and 19. The velocities far from the wall are used instead of the values just before impact due to the influence of squeeze-film damping, as described in Chapter 2.3.4.

$$\text{CoR}_n = \left| \frac{V_{n3}}{V_{n0}} \right| \quad (18)$$

$$\text{CoR}_t = \frac{V_{t3}}{V_{t0}} \quad (19)$$

$$\theta_i = \tan^{-1} \left(\frac{V_{n0}}{V_{t0}} \right) \quad (20)$$

The collision of an irrotational sphere with a flat plate, with constant material properties, can be fully described by three values: impingement angle θ_i , Equation 20; initial total velocity far from the wall V_0 and particle diameter D_p . The effects of temperature can be incorporated into the material properties

as described in Chapter 2.3.7, while surface roughness modifies the effective angle of incidence as described by Chapter 2.3.6. Equally, the rebound can be fully described by: CoR_n ; CoR_t ; and Ω . Where CoR_n is equal to zero, the particle is assumed to have adhered to the surface. Various bounce stick models relevant to deposition in gas turbines are discussed below.

2.5.1 Critical Viscosity Models

As discussed in Chapter 2.3.7, the mechanical properties of a particle vary with temperature. Experimental data shows that the capture efficiency of incoming particles increases exponentially above a critical softening temperature (Crosby et al., 2008). This change in mechanical properties can be expressed through viscosity, where higher temperatures lead to a less viscous and therefore “sticky” particle. Senior et al., 1995 developed a semi-empirical fit of temperature and viscosity for particulates, based on composition of different minerals. The softening temperature T_s can be used to calculate a ‘critical’ viscosity, below which the particle will stick. Sreedharan et al., 2010 subsequently developed the critical viscosity model, which estimates a sticking probability P_s for each impact based on the temperature of a particle. The trend of sticking probability with temperature is shown by Figure 21, where particles are guaranteed not to stick at the lowest temperatures and certain to deposit at temperatures above T_s . The mole fractions of the minerals that comprise the particle are used to calculate the critical viscosity, which is compared with the viscosity of the particle at a given temperature as shown in Equation 21. At impact, a random number between zero and one is compared with P_s to determine if the particle sticks.

$$P_s(T_p) = \frac{\mu_{\text{crit}}}{\mu_{T_p}} \quad (21)$$

When implemented in CFD, predicted capture efficiencies match data from coupon impaction experiments (Sreedharan et al., 2010). Singh et al., 2015 combined the critical viscosity approach with their more deterministic model for predicting coefficients of restitution (Singh et al., 2013), discussed further in Chapter 2.5.5. On the assumption that reductions in CoR imply collision energy loss and a greater chance of sticking, the predicted CoR_n is converted to an additional sticking probability $P_e = \exp(-6.5\text{CoR})$. The coefficient 6.5 is chosen on the assumption that the probability of deposition is only significant once the particle has lost more than half of its initial kinetic energy. To the

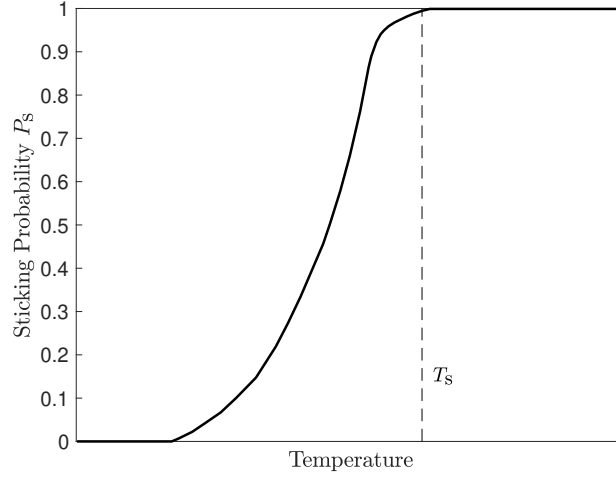


Figure 21: A schematic of sticking probability P_s of a particle vs. temperature, with reference to the particle softening temperature T_s . From Sreedharan et al., 2010.

author's knowledge, there is no physical or empirical justification for this assumption. This energy-based sticking probability is combined with that from the critical viscosity model, Equation 21, to form a total sticking probability P_{tot} :

$$P_{\text{tot}} = \min \{P_s + P_e, 1\} \quad (22)$$

Including the total CoR sticking probability allows tangential motion to influence deposition. Tangential motion, sliding or rolling, may influence the formation of the adhesive bond between particle and surface, however it is unclear if that is captured in the underlying physics of Equation 22. Singh et al. show that the model, when implemented in CFD, is able to capture the qualitative trend of capture efficiency with temperature although more specific validation is needed where the results are decoupled from CFD.

2.5.2 Critical Velocity Model

The model presented by Brach et al., 1992 uses an assumption of Hertzian contact coupled to the JKR theory of adhesion to predict the CoR_n of spherical particle-wall collisions. The model also presents a relation between tangential impulse and rebound angular velocity, however this requires the impulse of the collision to be known *a priori* and hence does not allow predictions of CoR_t and Ω for novel

collision cases. The rebound normal velocity V_{n3} is approximated using the work of adhesion W_A and e_0 , the CoR_n in the absence of adhesive and inelastic effects. While the physical significance of e_0 is not discussed by Brach et al., it amounts to a viscoelastic term due to its reliance on collision velocity (see Chapter 2.3.4). The normal rebound velocity can therefore be approximated as:

$$V_{n3} = -e_0 V_{n0} \left(1 - \frac{2W_A}{e_0^2 m V_{n0}} \right)^{\frac{1}{2}} \quad (23)$$

where W_A is positive. The analytical nature of the model, notably the reliance on Hertzian collision physics and the JKR theory of adhesion, leads to highly accurate predictions of CoR_n once e_0 is fitted to experimental collision data. The inability of the model to consider plastic deformation reduces accuracy at high velocities, while the flattened contact pressure distribution during inelastic compression will also invalidate the assumption of Hertzian contact. This would likely only occur where low yield stresses coincide with high surface free energies, for example where a variable yield stress is used as a non-physical fitting parameter. Where there remains a tangential slip velocity between the particle and wall throughout contact, a collision in gross-slip, the friction coefficient μ and impulse ratio are identical. This allows an analytical solution for the tangential velocity at rebound:

$$V_{t3} = V_{t0} - \mu (V_{n0} + V_{n3i}) \left(\frac{V_{n3}}{V_{n3i}} \right) \quad (24)$$

where V_{n3i} is the normal rebound velocity while neglecting adhesion. However, Equation 24 is unable to capture the tangential compliance of the contact patch or the transition to particle rolling, so is not accurate for highly normal collisions.

2.5.3 The Ohio State University (OSU) Model

The model proposed by Bons et al., 2017 aimed to provide the most physics-based approach to date when modelling rebound. The particle is treated as a 1D cylindrical spring with a constant stiffness and an empirical correction to allow for spherical geometry. As with the Thornton and Ning model in Section 2.3.5, the contact time is divided into three stages: elastic compression, plastic compression and adhesive-elastic rebound. Following first contact the particle deforms elastically, storing kinetic energy as elastic potential energy. Following the initiation of plastic deformation, all further deformation is

assumed to result in plastic work and no further elastic energy is stored in the particle. During rebound, the stored elastic energy is converted back into kinetic energy. Plastic deformation is assumed to start once a critical normal deformation is reached, $\delta_y = \sigma_y l / E^*$ where l is the length of the cylinder and E^* is the composite elastic modulus. Therefore, the energy available for rebound is expressed by the potential energy stored in the spring at the point of yielding, Equation 25.

$$E_{\text{crit}} = \left(\frac{E^* A}{l} \right) \frac{\delta_n^2}{2} \quad (25)$$

If the work of adhesion from JKR theory is greater than this stored potential energy, the particle remains adhered to the surface. If rebound occurs, the energy balance can be used to predict the CoR_n . Bons et al. suggest multiplying W_A by $\sin \theta_i$ to account for the influence of tangential impulse on adhesion. This is shown to improve model accuracy when compared to experimental data, however in the absence of empirical evidence for this correction is it also possible that the sine term is actually correcting for the “semi-empirical” contact area correction. The contact area correlation to convert between cylindrical and spherical geometries for a given normal deformation over-predicts area at low normal velocities by an order of magnitude compared to the Hertzian approach. Therefore, the sine term is artificially reducing contact area where it has the most influence: low normal velocities (i.e. oblique collisions).

The tangential coefficient of restitution is modelling using the same basic approach as Brach et al., with an additional $\cos^2(\theta_i)$ term to allow recovery of the CoR_t at high impingement angles (Equation 26). The justification for this is to account for decreased tangential engagement of asperities at normal impingement angles, however the recovery of CoR_t at high θ_i in experimental data where surfaces are smooth implies that it instead mimics tangential compliance of the contact patch:

$$V_{t3} = V_{t0} - \mu (V_{n0} + V_{n3i}) \left(\frac{V_{n3}}{V_{n3i}} \right) \cos^2(\theta_i). \quad (26)$$

The OSU model demonstrates accurate predictions of CoR_n and CoR_t where the input parameters can be tuned to experimental data. Whitaker et al., 2018 present an improved model that accounts for strain rate effects through a variable yield stress and stochastic corrections for particle shape. The

parametric approach to modelling non-sphericity may self-incorporate a number of physical phenomena, particularly when it is based on a fundamental method that requires fitting to data. It is therefore limited to the particle sizes, shapes, velocities and possibly flowfields tested (given the potential distributions of particle orientations near the wall). The amount of experimental data required to fit an approach for generic collisions of even a single material pair are likely prohibitive.

2.5.4 EBFOG

The Energy-Based Fouling Model for Gas Turbines (EBFOG), proposed by Casari et al., 2017, relates the particle sticking probability to the total particle energy at impact. This explicitly includes the effects of temperature, fitted to experimental collision data. Designed for high-temperature impacts, it is well suited to modelling deposition in the hot gas path which has been its primary application in literature thus far (Ellis et al., 2021; Casari et al., 2017; Suman et al., 2019). The model assumes that increased kinetic energy flux normal to the surface, including the thermal energy of the particle, will increase the likelihood of deposition. Casari et al. propose an Arrhenius-type equation (Equation 27) to predict the sticking probability P_s , analogous to the relationship between molecular energy and reaction rate in chemistry.

$$P_s = A \exp\left(\frac{-E_{\text{act}}}{E_{\text{case}}}\right) = A \exp\left(\frac{-2C_1}{m V_{n0}^2 (1 + C_2 T/T_s)}\right) \quad (27)$$

In Equation 27, A , C_1 and C_2 are empirical constants while T_s is the particle softening temperature. The numerator of the exponential is the activation energy of the process, above which sticking is likely and the denominator is effectively a reference energy for each case. The larger the denominator, the more likely the particle is to adhere. When relevant experimental data are plotted nondimensionally, Casari et al. demonstrate that they collapse to a curve. The EBFOG model therefore represents a close fit of high temperature deposition. However, the sticking probability does not capture the increased probability of deposition due to van der Waals adhesion at low impact velocities, even at low temperatures. It is therefore best suited to high temperature deposition of large particles in the hot gas path where either the particle is molten, or capillary forces are much greater than those from adhesion. The EBFOG model also does not predict the rebound properties of the particle, which will result in particle tracking errors where repeated impacts of the same particle occur.

2.5.5 Virginia Tech Deterministic Models

Critical viscosity methods developed by Danesh Tafti at Virginia Tech are discussed in Chapter 2.5.1. These models are highly empirical and unable to predict the rebound trajectory of impacting particles. Further work by Tafti and colleagues has developed a series of increasingly complex deterministic models that allow predictions of particle CoR and rebound angular velocity. First presented by Singh et al., 2013, an impulse-based approach was shown to produce accurate predictions of CoR_n considering plastic deformation and adhesion. The Jackson-Green model of plastic deformation is used to calculate the rebound velocity in the presence of only plastic deformation. Singh et al. then consider adhesive losses separately using JKR theory, based on the approach developed by Brach et al., 1992. The approach was the most comprehensive overview of the physics to date, although experimental validation was limited. The most recent model was presented by Yu et al., 2019 which includes the effects of surface roughness on plastic deformation and adhesive losses for the first time in open literature. The model also includes viscoelasticity using an empirically-derived coefficient. Tangential rebound is calculated assuming an empirical coefficient of friction that varies significantly with impact angle, contrasting from an earlier approach by Yu et al., 2017 which applied a deterministic, rigid body approach to calculating Ω and CoR_t . The current model was mostly validated using only total CoR so it is difficult to compare with results for other models that report CoR_n and CoR_t separately. The results presented show reasonable agreement to experimental data, however further validation is needed before use in CFD.

2.6 Deposition Evolution & Detachment

If deposition models are to be routinely used in design, how the deposits evolve and shed with time must be known to predict the effect on component performance. While deposit evolution and shedding are not within the scope of this research, understanding the effect of prior deposition is important to interpret experimental deposition data and specify an appropriate bounce stick model.

A qualitative understanding of volcanic ash deposition can be gained from Giehl et al., 2017, which recorded the deposition, evolution and detachment of particles on a nickel-alloy coupon. Particles that ranged from $5\mu\text{m} - 500\mu\text{m}$ in diameter were heated in an acetylene torch which also acted to propel them towards the coupon that was kept at 1250°C . While some of these particles are much larger

than those that would be found in the secondary air system, the largest particles' thermal inertia cause them to bounce rather than stick and have a small effect on the qualitative results of the study. There were three main stages to the deposit evolution, listed below with some shown in Figure 22:

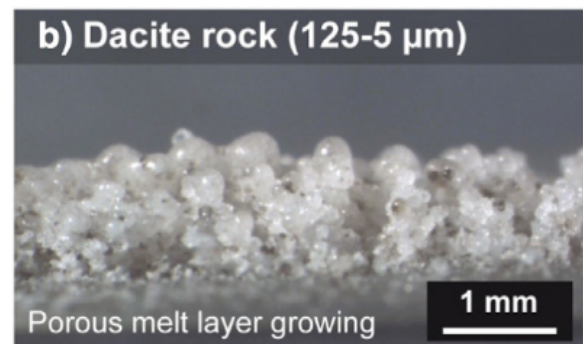
- A 'cindery' deposit would form when the first particles impact the surface, where the particles quench to a dull finish with an angular or round form.
- Porous melts, which form rounded and shiny deposits where crystal structures are sometimes visible. These particles typically form on top of cindery deposits, being insulated from the cooling coupon surface.
- A 'melt bath' forms from coalesced molten particles, typically on top of other deposits.

Once the acetylene torch is switched off and the coupon cools, the differing coefficients of thermal expansion between the nickel alloy and ash particles cause stresses that fracture and dislodge large parts of the deposit. The evolution process is shown in Figure 23, albeit without detachment explicitly shown.

When modelling deposit growth in CFD, an evolution and erosion model would need to modify the mesh to account for the effect of the deposition on the flow field. One approach is to use dynamic mesh morphing, as in Forsyth et al., 2017. First, new boundary node coordinates are calculated from the volume of particles deposited at each node, based on the mass flow rate per deposited particle integrated with a pseudodeposition exposure time. The deposited material is then distributed between different nodes to reduce the likelihood of a 'spiky' mesh with an irregular surface; in effect, smoothing.



(a) Initial stages of Basalt rock deposition with particle-particle impacts



(b) Development of the porous melt layer of Dacite rock

Figure 22: Close-up images of deposit evolution, Giehl et al., 2017

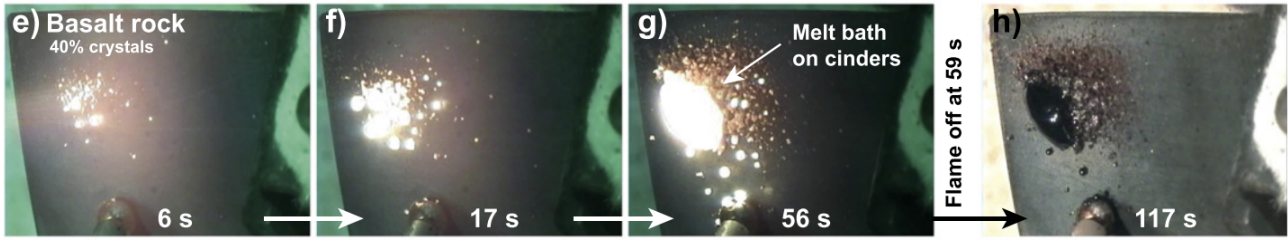


Figure 23: Deposit evolution of Basalt rock, starting with cindery deposits, progressing to a porous melt and melt bath, Giehl et al., 2017

If deposition has occurred at a node - according to the user-defined deposition model - then the nodal displacements are calculated from the deposit volume. Built-in dynamic meshing functions are then used to update the volume mesh from the nodal displacements: boundary layer deformation was used as it allowed the greatest displacements while retaining the prism layer structure near the wall. The model was used to simulate the blockage of film cooling holes in comparison with experimental data. The geometry is shown in Figure 24 with a qualitative comparison of results in Figure 25.

Due to mesh constraints, the fine structures seen in Figure 25b were not replicated in Figure 25a. However, the essential shape and magnitude of the deposit were captured. Given that the OSU model was used throughout to simulate deposition, mesh morphing would be a credible approach to use with an improved bounce stick model for use in gas turbine design. An alternative approach was proposed by Connolly et al., 2018 which converts existing fluid cells to solids in order to build up a deposit. While the approach avoids some problems with the mesh morphing strategy like overlapping volumes, the process of identifying cells for the transformation is significantly slower than mesh morphing.

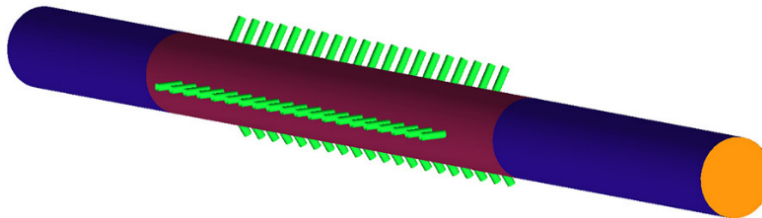
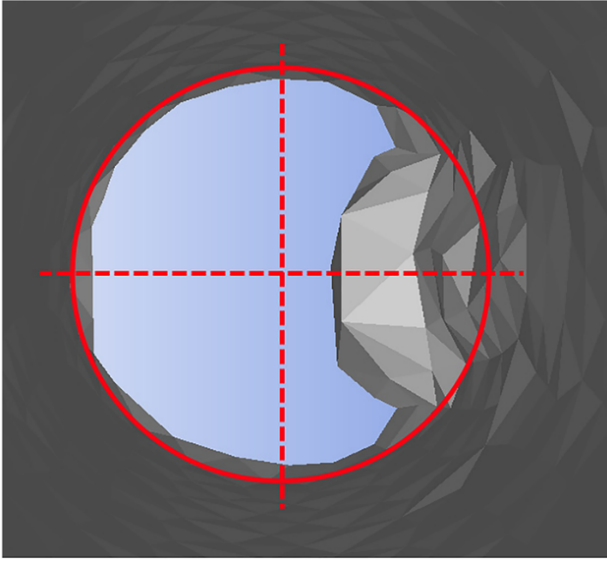
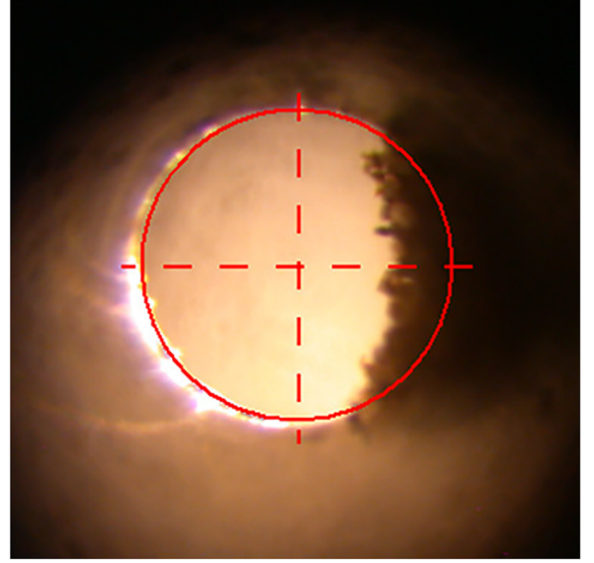


Figure 24: The computational domain from Forsyth et al., 2017. Flow is right to left and exits through the film cooling holes shown in green



(a) Numerical simulation of film cooling hole blockage



(b) Experimental blockage of a film cooling hole

Figure 25: Comparison between experimental and numerical film cooling hole blockage, from Forsyth et al., 2017.

2.7 Discrete Element Methods

Discrete Element Methods are a family of explicit time-stepping schemes that track individual particles. The forces that act on particles are calculated at each time step and the equations of motion integrated, hence the velocities and displacements of the particle can be found. Forces can originate from interactions between the particle and fluid phase, particles and other solid bodies, particles and other particles and body forces like gravity. Where only particle-fluid interactions are relevant, the DEM approach amounts to Lagrangian particle tracking. DEM approaches are most often used where non-fluid forces dominate particle motion. Generally, simulations of large granular assemblies like grain silos (Kobylka et al., 2014; Xu et al., 2002), the 3D printing of powders (Sen et al., 2021), and geological phenomena like landslides (Lu et al., 2014; Camones et al., 2013). A variety of models exist in the literature for modelling particle-particle and particle-surface forces. These are generally divided into those that model normal and tangential forces, with respect to the collision plane (the collision surface, in the case of a particle-surface impact). The choice of tangential force model is generally independent of normal force model, however the accuracy of the normal model will influence tangential modelling. For example, modelling simple Coulomb friction during sliding relies on the normal force between the particle and surface. However, the formation of normal and tangential

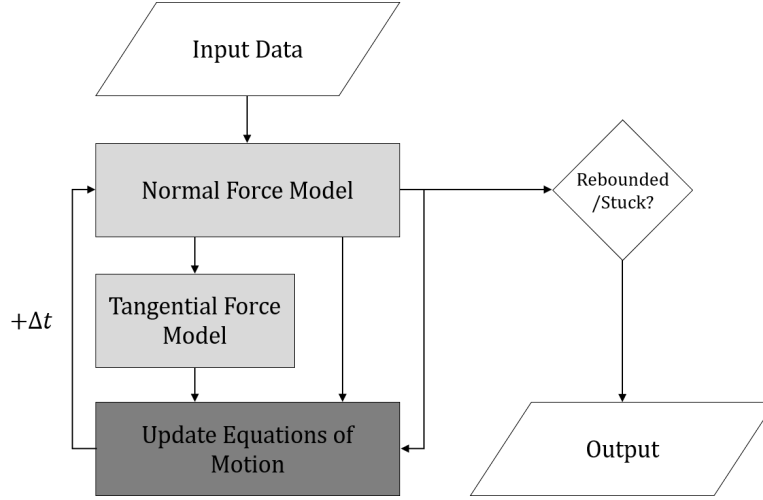


Figure 26: Flowchart showing the DEM explicit process.

contact stresses are fundamentally decoupled allowing them to be modelled sequentially within a single timestep (Kruggel-Emden et al., 2008). A flowchart that describes the DEM process is shown in Figure 26. Input parameters - material properties and collision data like impact velocity - are fed into an explicit time-stepping loop that continuously updates the equations of motion. At each time step, whether the particle has rebounded is checked and the simulation is terminated accordingly.

Thornton et al., 2017 analysed the performance of different adhesive, plastic normal force models. Contact mechanics-based models from Thornton et al., 1998 and Martin, 2003 were compared to the simpler piecewise linear approaches from Luding, 2005 and Pasha et al., 2014. DEM normal force models predict the stiffness of the particle as it deforms k_n , with the normal force between contacting surfaces obtained in conjunction with the incremental normal overlap $\Delta\delta_n$:

$$F_n(t + \Delta t) = F_n(t) + k_n \Delta\delta_n. \quad (28)$$

Both contact mechanics-based models assume a truncated Hertzian pressure distribution as described by the FEA simulations presented in Wu et al., 2003, Figure 12. This assumption is what leads to the constant loading stiffness demonstrated by the normal force curve diverging as the tangent of the Hertzian solution in Figure 13. Both models assume the JKR model of adhesion, with Thornton et al. applying adhesive forces during loading and Martin assuming rebound only. This makes the model presented by Martin inappropriate for more general collision problems where adhesive forces

are dominant, for example agglomeration (Thornton et al., 2017). The approach to modelling plastic deformation matches experimental data from Wall et al., 1990 and the theoretical dependency on collision velocity: $\text{CoR}_n \propto V_i^{-0.25}$. The piecewise linear models assume constant contact stiffnesses at all stages of contact (elastic deformation, plastic deformation and elastic-adhesive unloading). This leads the models to end contact when the relative approach returns to zero at rebound, ignoring that plastic deformation permanently deforms the contact patch. This leads to the models being unable to predict the limiting case $\text{CoR}_n \rightarrow 0$ as $V_i \rightarrow 0$. Upon inspection of the models, they also predict that $\text{CoR}_n \propto V_i^{-0.5}$, contrary to the negative quarter power law that is well established by theory (Thornton et al., 2017) and experimental data (Wall et al., 1990). The normal force model presented in Thornton et al., 1998 therefore provides the most physical representation of normal contact stiffness.

Several different approaches are taken in literature to modelling tangential compliance, summarised by Kruggel-Emden et al., 2008. Early work by Mindlin et al., 1953 was implemented by Maw et al., 1976, discretising the contact patch into concentric annuli that exist in either gross-slip or gross-stick with a colliding surface. The full integral version proposed by Mindlin et al., 1953 was simplified by Di Renzo et al., 2005 and implemented in DEM, albeit with significant computational cost. A model proposed by Brilliantov et al., 1996 assumes that tangential force is transferred between contacting surfaces by the interaction of asperities. When exceeding a certain local stress, the asperities fracture which leads to a macroscopic shift between the surfaces. The asperity-based approach leads to a saw-tooth profile of tangential force with time, as the force rapidly oscillates between the Coulomb limit and zero friction. According to Kruggel-Emden et al., this arguably non-physical phenomenon leads to “strong and constant deviation from the experimental results”. Other models are based on the assumption of a tangential spring between the bulk of the particle and the contact patch, where the total frictional force is restricted by the Coulomb limit. Some models, notably the earliest implementation of this model by Cundall et al., 1980, prescribe an unconstrained tangential spring, while others like Di Maio et al., 2004 limit the spring’s elongation. In practice, the extension of the spring will be self-limiting as the moment the tangential force exerts about the particle centroid increases the angular velocity to the point of a zero or negative slip velocity between the particle and the surface. This is shown by the governing equation of the model presented by Cundall et al. in Equation 29, where the tangential

spring extension δ_t is the time integral of the slip velocity between the particle and surface V_s . Note that Equation 29 also includes a viscoelastic dissipation term which was not included in the original implementation by Cundall et al.

$$F_f = \min [|k_t \delta_t + \eta_t V_s|, -\mu |F_n + 2F_c|] \quad (29)$$

Figure 27 shows schematic representations of the tangential force that acts on the contact patch throughout a collision. Figures 27a to 27c refer to a constrained spring while Figures 27d to 27f refer to an unconstrained spring. The reversing polarity of the force throughout the contact time at large and intermediate impingement angles demonstrate the importance of including tangential compliance. Assuming sliding throughout contact would lead to significant errors in tangential rebound and angular velocity when considering that tangential impulse is the time integral of the graphs in Figure 27. In comparison with experimental data, Kruggel-Emden et al. showed that constrained spring models provided the best accuracy.

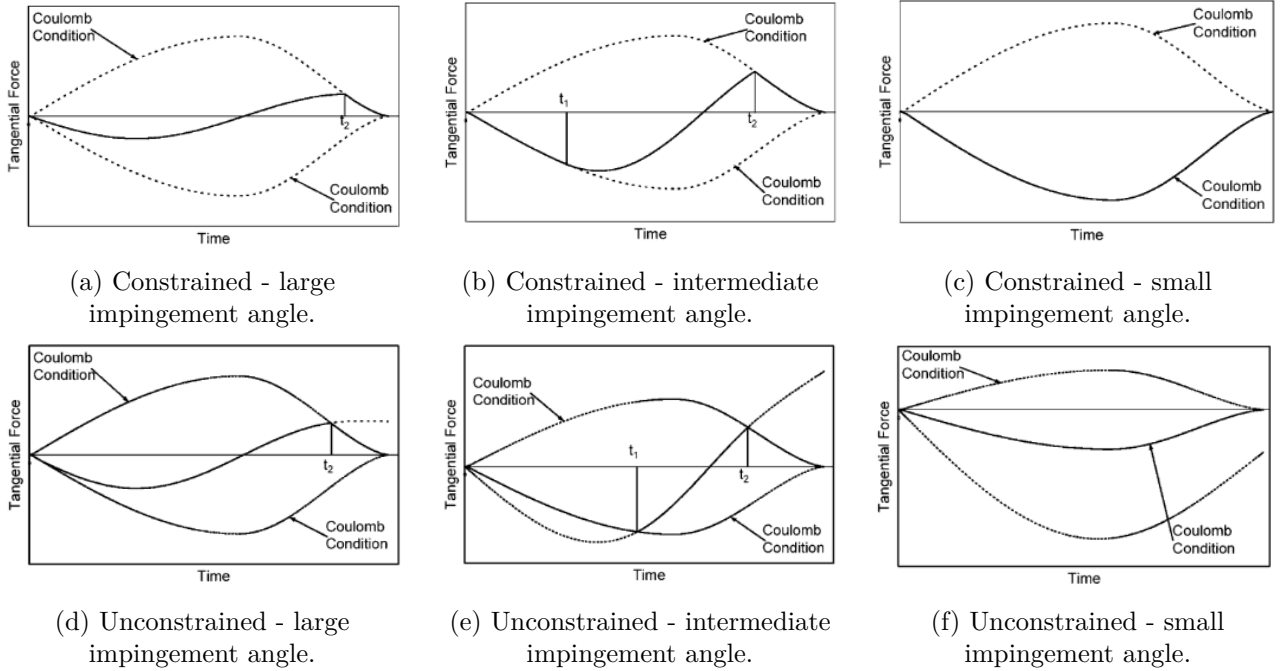


Figure 27: Schematic representations of tangential contact forces for constrained and unconstrained tangential springs, from Kruggel-Emden et al., 2008.

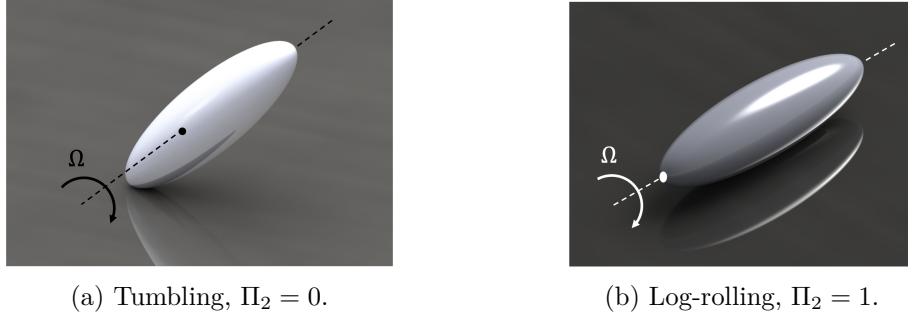


Figure 28: Schematic of prolate spheroid rotation modes: tumbling and log-rolling. The axis shown is the vector of the axis of rotation, Ω . The rotation parameter Π_2 is defined in Equation 32.

2.8 Non-Spherical Particle Transport

As discussed in Chapter 2.2, particles ingested by the gas turbine are likely to be non-spherical. Tracking spherical particles in turbulence already presents significant challenges, as discussed in Chapter 2.4. The additional challenge of anisotropy is described by Voth et al., 2017 as “quite complicated”: orientation-dependent forces and torques are, themselves, dependent on shape, initial orientation, and fluid and particle inertia. Marchioli et al., 2010 found through DNS that long fibres exhibited a higher wall-ward drift velocity in turbulent channel flow than spherical particles. In real systems, this is likely to increase deposition for non-spherical particles. This conclusion is echoed by many other workers in the literature (Gavze et al., 1998; Parsheh et al., 2005; Carlsson et al., 2010). Both prolate and oblate spheroids are also known to segregate into low speed streaks near the wall, with the degree of segregation increasing with particle inertia (Voth et al., 2017).

Jeffery, 1922 describes the motion of rigid, inertia-less spheroids in Stokes flow, subject to mean shear. The behaviour of particulates in mean shear is particularly relevant in the context of bounce stick modelling, due to the similarity with flow in the viscous sublayer, near the wall. A spheroid’s axis of symmetry was found to perform periodic motion on an infinite number of closed orbits, known as “Jeffery” orbits. The orbit results in the minimum dissipation of energy, dependent on initial orientation. Jeffery’s theory of closed orbits has been experimentally validated (Mason et al., 1956; Trevelyan et al., 1951), however it is limited to cases with negligible fluid and particle inertia. In 2D Stokes flow, the prolate spheroids are shown to tumble with the angular velocity:

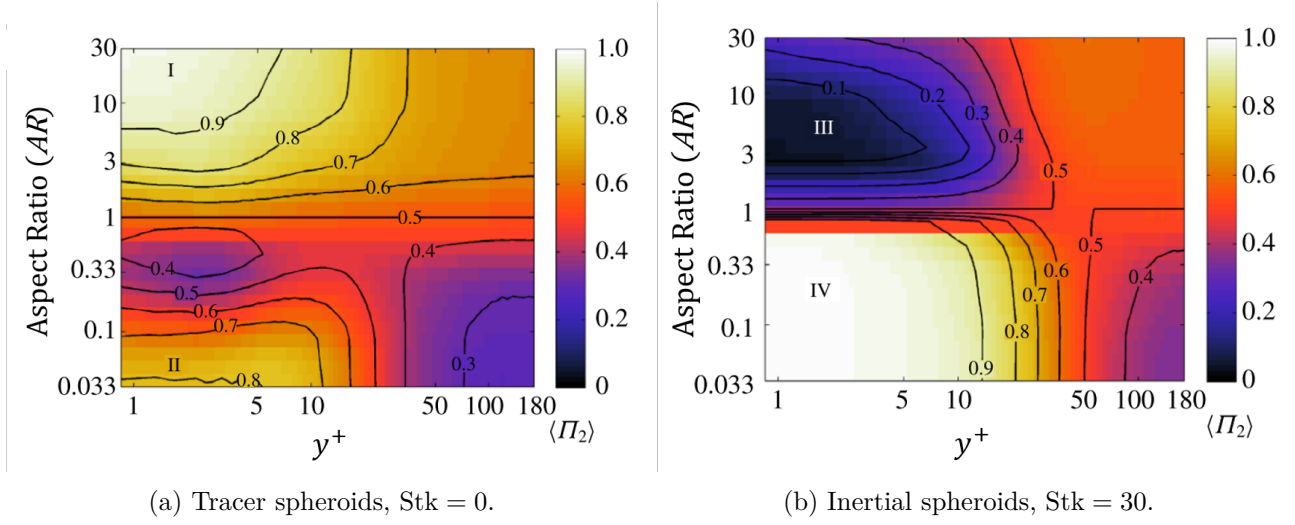


Figure 29: Contour plot showing the rotation parameter $\langle \Pi_2 \rangle$ for (a) inertialess spheroids $\text{Stk} = 0$ and (b) inertial spheroids $\text{Stk} = 30$. Stokes number, Stk , is defined in Equation 13. $\langle \Pi_2 \rangle$, defined in Equation 32, represents particle orientation relative to particle rotation. $\Pi_2 = 0$ represents tumbling while $\Pi_2 = 1$ represents log-rolling. Figure from Zhao et al., 2019.

$$\Omega = \dot{\theta} = \frac{1}{\text{AR}^2 + 1} \left(\frac{1}{2} (\text{AR}^2 - 1) \sin(2\theta) \left(\frac{\delta u_y}{\delta y} - \frac{\delta u_x}{\delta x} \right) + (\sin^2(\theta) + \text{AR}^2 \cos^2(\theta)) \right. \\ \left. \frac{\delta u_y}{\delta x} - (\cos^2(\theta) + \text{AR}^2 \sin^2(\theta)) \frac{\delta u_x}{\delta y} \right) \quad (30)$$

as expressed by Olson et al., 1998. Note that u is the fluid velocity and θ is the orientation of the particle with respect to a fixed axis. Initial verification of Jeffery's theory was performed by Taylor, 1922, who noted that while the initial orbits observed experimentally matched theoretical predictions, the aluminium particles eventually settled to a preferred orientation. It was noted that this behaviour was likely to be due to inertial terms neglected in Jeffery's analysis. The development and advancement of computational methods have since allowed detailed studies of single particles immersed in shear flow. Neutrally-buoyant prolate spheroids were shown by Qi et al., 2003 to drift towards an orbit involving preferential orientation in the shear plane, so-called "tumbling". Inertial spheroids in shear flow were studied by Mao et al., 2014 using a lattice Boltzmann method. Prolate spheroids with an arbitrary initial orientation drifted towards tumbling at small particle Reynolds numbers (Re_p), as defined by the shear rate, with a constant angular velocity. When initially orientated in the shear plane, Reynolds numbers above a critical value induced settling at a constant orientation with respect to the flow, with

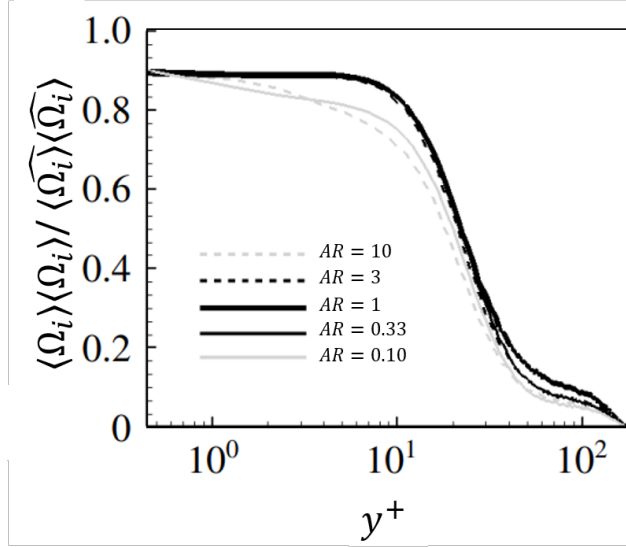


Figure 30: Ratio between mean particle angular velocity $\langle \Omega_i \rangle \langle \Omega_i \rangle$ and fluctuating particle angular velocity $\langle \hat{\Omega}_i \rangle \langle \hat{\Omega}_i \rangle$ for inertial particles $\text{Stk} = 30$. Figure from Zhao et al., 2019.

zero angular velocity. Increasing fluid inertia up to this point increased the rotational period, i.e. decreasing the angular velocity at which the particle tumbled. Streamlines in the shear plane for Stokes flow and finite Re_p showed qualitative differences, with regions of recirculation on either side of the particles. With arbitrary initial orientation, prolate spheroids tended towards log-rolling with large fluid inertia ($Re_p \approx 60$).

The rotation modes of non-spherical particles throughout turbulent channel flow was mapped by Zhao et al., 2019 using DNS-based Eulerian-Lagrangian simulations. This allows the results from single particle simulations, discussed above, to be interpreted in the context of an engineering-relevant system. The position of particles relative to the wall is defined by the dimensionless wall distance y^+ , given in terms of the actual distance from the wall y :

$$y^+ = \frac{u^* y}{\nu_f} \quad (31)$$

Significant differences were observed between distinct wall and centre rotation modes. The transition between these two regimes was observed at $y^+ \approx 40$, where the spheroids were inertial. This is attributed to the point where the Kolmogorov time scale becomes comparable to the particle period of rotation. By contrast, tracer spheroids transition closer to the wall, $15 < y^+ < 35$, due to the changeover between mean shear and small scale turbulence time scales. As expected from the simu-

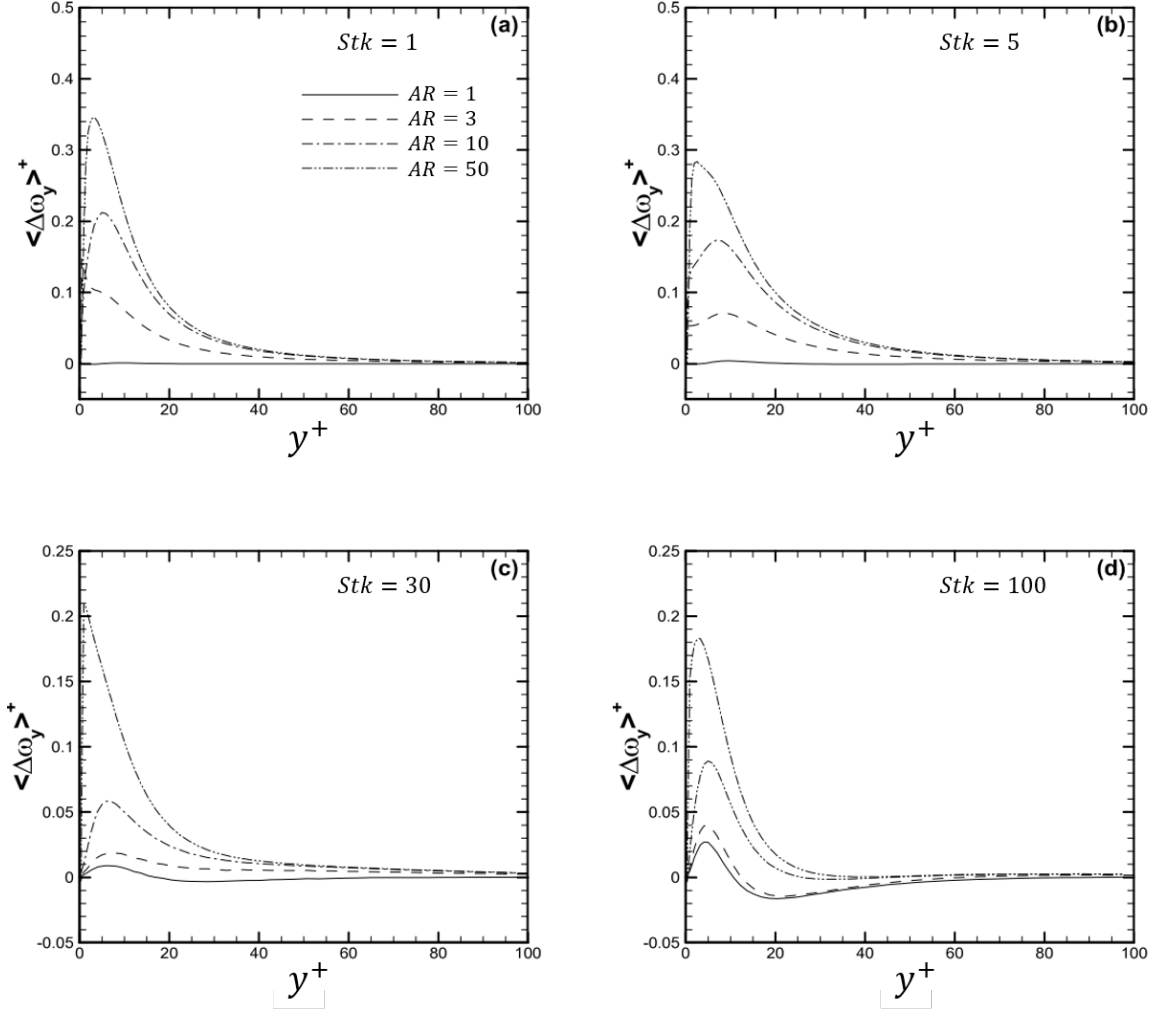


Figure 31: The effect of particle inertia, shape and wall-normal distance on angular slip velocity $\Delta\omega_y^+ = \Omega_y^+ - \omega_y^+$, where ω_y^+ is the fluid rotation rate vector. Figure from Marchioli et al., 2016.

lations of single particles, discussed above, inertial prolate spheroids close to the wall in mean shear preferentially tumble. A schematic of tumbling is shown in Figure 28a. Figures 29a and 29b show the behaviour of spheroids at different non-dimensional wall distances, for tracer and inertial particles respectively. Rotation is expressed using the rotation parameter $\langle \Pi_2 \rangle$, which represents the particle's major axis vector $\bar{p}$ with respect to its axis of rotation $\bar{\Omega}$:

$$\Pi_2 = \frac{\bar{p} \cdot \bar{\Omega}}{|\bar{p}| |\bar{\Omega}|}. \quad (32)$$

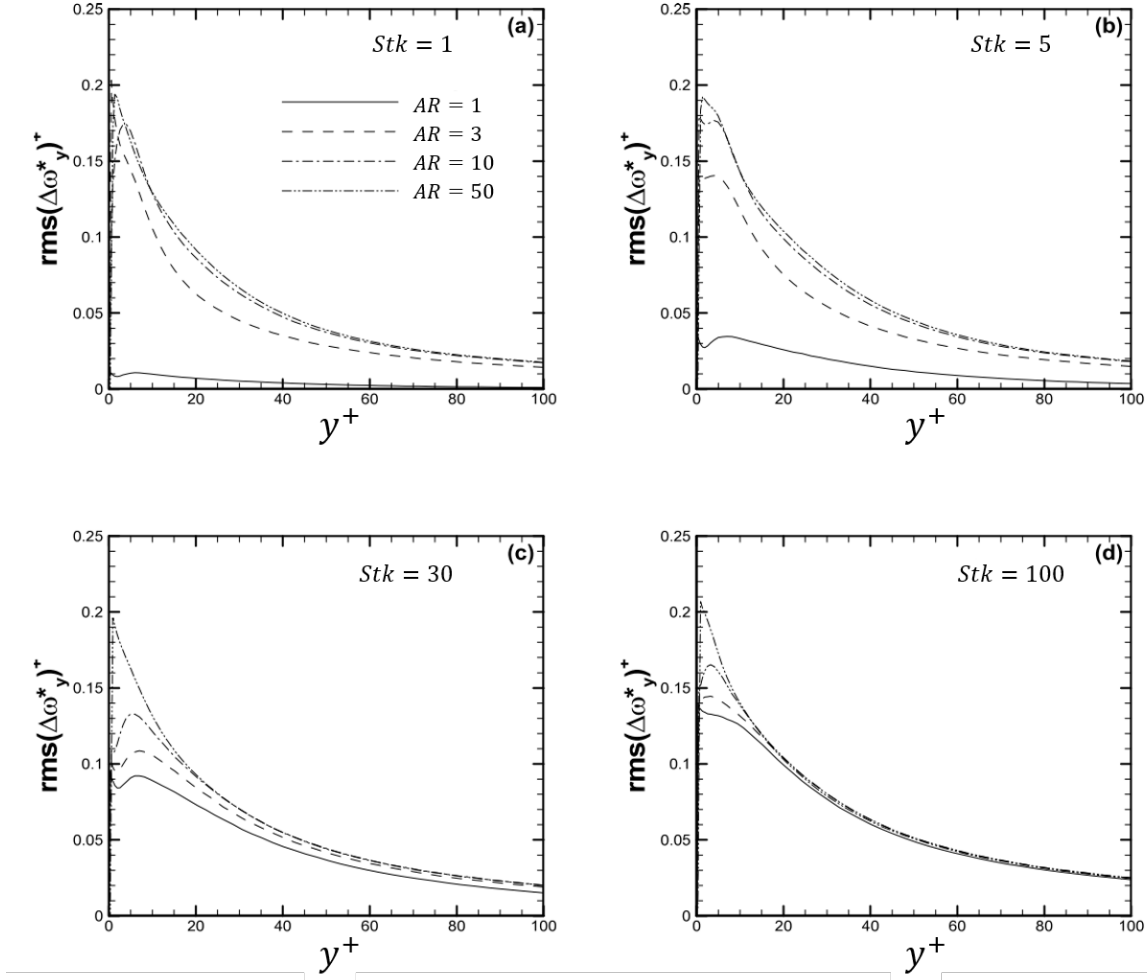


Figure 32: The effect of particle inertia, shape and wall-normal distance on RMS fluctuations of angular slip velocity $\Delta\omega_y^+ = \Omega_y^+ - \omega_y^+$, where ω_y^+ is the fluid rotation rate vector. Figure from Marchioli et al., 2016.

Where $\Pi_2 = 0$, the particle is tumbling while $\Pi_2 = 1$ represents log-rolling. Log-rolling is shown schematically in Figure 28b. In the absence of particle inertia, prolate spheroids (aspect ratio $AR > 1$) preferentially log-roll near the wall with random orientations towards the channel centre. Inertial prolate spheroids display different qualitative behaviour, tumbling at less than $y^+ \approx 15$. A sharp transition is observed around $AR = 1$, with oblate spheroids tumbling in the same region. The difference between inertial and tracer spheroids indicates that drag dominates particle dynamics where a mean slip velocity exists: Njobuenwu et al., 2015 describe how a moment is induced by the displacement between the centre of pressure and centre of mass. The angular velocity at which the prolate spheroids tumble is relatively constant, as shown by the ratio between mean and fluctuating components of particle angular kinetic energy near the wall in Figure 30. This contradicts results from similar studies,

discussed later. The particle dynamics described by Zhao et al. indicate that, in turbulent channel flow, the slip velocities experienced by inertial particulates are not sufficient to produce the transition to log-rolling at $Re_p \approx 60$, as seen in single particle simulations. They note that “particle dynamics in the vicinity of a wall is similar to the behaviour in a simple shear flow, in which inertia was found to drive a particle to align in the velocity-gradient plane”. This conclusion is echoed by Challabotla et al., 2015; Lundell et al., 2010.

The angular slip velocity between the particle and fluid was studied by Marchioli et al., 2016. Near the wall, particles were found to spin more slowly than the fluid. The non-dimensional slip velocity was characterised as $\Delta\omega_y^+ = \Omega_y^+ - \omega_y^+$, where ω_y^+ is the fluid rotation rate vector. The mean angular slip velocity with varying Stokes number and shape is given in Figure 31. A particle with higher inertia tends to more closely follow the mean rotation of the fluid, with greater deviations as the particle becomes increasingly non-spherical. A prolate spheroid with aspect ratio $AR = 3$ has, on average, only a 5 % deviation from the local fluid rotation. It can be shown analytically that a tracer sphere in Stokes flow will rotate at half the fluid vorticity (Parsa et al., 2011). The RMS fluctuations of angular slip velocity are shown in Figure 32. While the angular slip of a spherical particle becomes increasingly unsteady with greater inertia, the behaviour of fibres is relatively consistent. Greater fluctuations of angular slip are explained by Equation 30, which describes a periodic angular velocity defined by the fluid strain and particle orientation. This contradicts the findings of Zhao et al., 2019 in Figure 30, however it is unclear what averaging window was used to calculate the fluctuating components in that case. If fluctuating kinetic energies are compared between periods greater than the rotation timescale, it is possible for both Figure 30 and Figure 32 to be correct. However, the agreement between the low Stokes number case in Figure 32a and the analytical result from Equation 30 implies that the angular velocity of a prolate spheroid will vary periodically throughout a rotation cycle.

To summarise, a prolate spheroid in turbulent channel flow is most likely to tumble when near the wall. The mean angular velocity at which a particle with aspect ratio $AR \leq 10$ will tumble is $\mathcal{O}(10\%)$ lower than the rotation rate of the local fluid. This angular velocity is periodic and can be expressed for

the case with negligible fluid and particle inertia using Equation 30. Results from DNS by Marchioli et al. indicate that this periodicity is similar for highly inertial particles, based on the similarity of RMS angular slip velocities for a variety of Stokes numbers.

3 Collision-Induced Rotation and the Magnus Force on Particulates

The paper presented below describes the influence of the post-collision angular velocity of particulates on their subsequent trajectories. The work was conducted to challenge the assumption, popular in gas turbine particle tracking literature, that the Magnus force can always be neglected. The results of this paper drove the inclusion of angular velocity as an essential output of bounce stick modelling, described in later chapters. More fundamentally, it provided the first demonstration of the importance of modelling particle rebound in addition to the binary bounce stick criterion. As a result of these findings, the bounce stick model developed in Chapter 5 placed equal emphasis on predicting rebound trajectories in addition to the binary bounce stick criterion.

This work was conducted prior to the development of an experimentally-validated bounce stick model, so includes the derivation of a low-order model to predict particle angular velocity and CoR_t . The effect of CoR_n is therefore neglected here. The results of the paper demonstrate that this may be important for the length of time the particle spends in the low velocity fluid in the boundary layer, leading the flow as it behaves ballistically. However, this is a second-order effect that has little influence on the main conclusions of the paper: that collision-induced rotation may influence rebound trajectories and hence should be included as an output of bounce stick modelling. Subsequent work in Chapter 5 has also demonstrated that the effects of rolling adhesion on CoR_t and therefore Ω are small, leading to confidence in the predictions of the low-order models presented. In Chapter 6, the quantitative and qualitative distribution of deposition predicted by CFD simulations changed significantly if CIR was excluded, validating the central conclusions of this paper.

These simulations were also conducted prior to the availability of a version of the CRW transport model for use with RANS turbulence models. The Discrete Random Walk (DRW) model, which is included in ANSYS Fluent 19.2, was used instead. When compared to the CRW, the DRW will over-predict particle deposition due to turbophoresis as described in Chapter 2.4. This may increase the likelihood of repeated collisions with the wall and hence the mass of particulate matter deposited. Therefore,

the relative effect of CIR on deposition compared to turbophoresis alone may be understated here. However, the qualitative effect and trend will still be representative of a real system.

The author of this report is the primary author of the paper and generated all the material reported, originally presented at the 2020 AIAA Aviation Forum. Professors Gillespie and McGilvray supervised the work while Dr. Rory Clarkson of Rolls-Royce offered helpful feedback on the applications of the work to gas turbine components. Nikul Vadgama, a DPhil candidate at the time of publication, helped with the implementation of the model in a Fluent User Defined Function (UDF).

Collision-Induced Rotation and the Magnus Force on Particulates

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The secondary air system and internal cooling passages of turbine blades have long been at risk from blockage through the deposition of sand and dust during fleet service life. Particles entering the cooling system which collide with the wall may bounce, stick or shatter on impact. While the effect of particle spin prior to impact due to fluid shear has previously been shown to be negligible, spin arising from impact has, to date, been neglected in particle modelling. Spin generates a Magnus force perpendicular to the direction of the slip velocity which modifies the trajectory of the particle. A deterministic low order model (LoM) of particle rebound rotation and tangential coefficient of restitution is derived in this paper and from this the Magnus force is quantified for a range of particle sizes and Stokes numbers. Particle tracking simulations are conducted on a secondary air system-representative duct with and without collision-induced rotation enabled to quantify changes in the downstream particle trajectory, including the likelihood of subsequent wall collisions and deposition. Collision-induced rotation increases deposition in this case with the magnitude of the increase dependent on particle diameter, Stokes number and fluid density. Instances were also recorded of up to 35% of injected particles depositing with rotation where no particles stuck without. The results demonstrate that rotation-induced lift may not always be neglected from particle tracking simulations where collisions occur.

Nomenclature

Roman Symbols

$F_{n,ave}^*$	Collision impulse, kg m s^{-1}
$\bar{U}_g$	Mean flow velocity, m s^{-1}
Δr_d	Change in the percentage of injected particles that deposit with and without collision-induced rotation
CoR_t	Tangential coefficient of restitution
D_h	Channel hydraulic diameter, m
E_{kt1}	Initial tangential kinetic energy, J
G	Shear modulus, Pa
I	Particle moment of inertia, kg m^2
m	Particle mass, kg
r	Particle radius, m
Stk	Particle Stokes number
t	Contact time, s

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t_{cont}	Contact duration, s
V_{∞}	Free stream velocity, m s^{-1}
$V_{\text{slip},f}, V_{\text{slip},w}$	Particle-fluid and particle-wall slip velocities, m s^{-1}
W_{slide}	Work done due to friction, J
E	Energy, J
F	Force, N

Greek Symbols

κ	Normal to tangential stiffness ratio at impact (Maw model)
μ	Coefficient of friction
μ_g	Fluid dynamic viscosity, $\text{kg m}^{-1} \text{s}^{-1}$
Ω	Particle angular velocity at rebound, rad s^{-1}
Ω_{max}	Maximum collision particle angular velocity - Equation 25, rad s^{-1}
ρ_p, ρ_f	Particle density and fluid density, kg m^{-3}
τ_p, τ_g	Particle relaxation time and flow characteristic time, s
θ_i	Particle impingement angle, $^{\circ}$
θ_{crit}	Critical angle between sliding and sticking regimes (Maw model), $^{\circ}$
ν	Poisson's ratio

Superscripts

*	Time-independent
'	Next instance of time-marching scheme

Subscripts

ave	Average
n	Wall-normal
t	Tangential to the wall

I. Introduction

Ingested particulates are known to cause significant damage to gas turbine engines. Previous work [1, 2] has demonstrated that erosion and deposition can cause cooling-passage blockage, corrosion and reduction in turbine capacity. Predicting deposition and erosion is desirable both to quantify the cost of ownership effects that arise from atmospheric contaminants and to allow the optimisation of component geometry to minimise engine deterioration.

Particulate modelling can be divided into two main bodies of work that have previously had little overlap: particulate transport and bounce-stick behaviour. Bounce-stick modelling focuses on the behaviour of the particle from contact with a solid surface to the point at which it either rebounds, sticks or shatters. Previous work in this area, notably [3–5], aims to predict coefficients of restitution for particles considering material properties, temperature and geometry. This allows individual sticking probabilities and trajectories to be calculated, influencing deposition where multiple impacts occur per particle. Particulate transport literature primarily focuses on the effect of turbulence and other fluid forces near the wall that influence whether collisions occur (notably [6, 7]). Existing literature assumes that lift due to the Magnus force is negligible, as lift from rotation due to fluid shear is much less than the lift induced by shear itself when the Reynolds number is small [8, 9]. However, other causes of particle rotation can produce a

significant Magnus force: it was shown to be the largest aerodynamic factor in the trajectory of saltating particles by [10, 11]. Creating an empirical model of saltation dynamics, [11] found that inclusion of the Magnus force increased particle horizontal displacement five-fold compared than with shear lift alone. Indeed its inclusion was necessary to match experimental data, concurring with [10] which also found that the maximum particle height reached by experiments was approximately 30% greater than possible with gravity alone, confirming the presence of a significant lift force.

The present research addresses two questions: can the rotation of spherical particles due to collisions with a wall be modelled and is the Magnus force that results from that rotation sufficient to affect particle trajectory in conditions relevant to gas turbines?

II. Magnus Force Modelling

The Magnus force on spinning particles with very small Reynolds numbers was solved analytically by [12], demonstrating that force is linearly dependent on the angular velocity, (Ω) , and slip velocity, $V_{\text{slip},f}$, of the particle within the flow:

$$\mathbf{F}_L = \pi r^3 \rho_f \Omega \times \mathbf{V}_{\text{slip},f} [1 + O(Re)] \quad (1)$$

From [13], $V_{\text{slip},f}$ and therefore lift has been shown to be highly dependent on particle Stokes number in wall-bounded turbulence. This is perhaps unsurprising as the magnitude of the mean $V_{\text{slip},f}$ tends to increase with Stokes number. In the bulk flow, the mean slip velocity is positive (i.e. the fluid leads the particle) while close to the wall in the boundary layer the sign of the slip velocity may reverse, depending on the particle trajectory. The flow field is more complicated close to the wall where the variance of the slip velocity is typically three to five times greater than the magnitude of the mean. Thus for where wall effects are significant a probabilistic model of the unsteady near wall velocity or the use of time-resolved simulations of the flow field may be necessary to predict particle tracking. None the less in this paper, where the size of the phenomena are being investigated time-averaged CFD is used. This conservatively demonstrates the overall effect of the Magnus force on particulates.

Previous workers [14] have developed a particle rotation model that is included in the commercial flow solver ANSYS Fluent 19.2 [15] to predict the angular velocity of particles provided the velocities before and after collision are known. The model considers the impulse on the particle during collision allowing angular velocities and coefficients of restitution to be calculated. As the rebound characteristics of particles are generally unknown *a priori*, it is not appropriate for use in the this paper. The model also fails to account for contact patch effects such as friction or elastic compliance which are known to be important in particle rebound dynamics [16]. Similar models of tangential coefficients of restitution from [3, 17] are generally impulsive and either only consider losses due to friction or use synthetic material properties that require all model predictions to be fitted to experimental data.

The key potential application of the present work is in better predicting the transport of particles in the jet engine secondary air system. Particles that exit the compressor train of a jet engine are typically around $6 \mu\text{m}$ in diameter [18], which are the focus of this study. In contrast, particles that enter the fan may be $> 100 \mu\text{m}$ [19], and while these are not modelled here, the approach is equally applicable to compressor erosion by these larger particles. To aid the prediction of particle rotation, a model of particle impact proposed by Maw et al. [16] is used as a basis to describe the frictional behaviour of a colliding elastic sphere and a semi-infinite half-space. The model does not consider adhesion in the manner generally considered elsewhere in the literature (i.e. using van der Waals forces) but instead considers friction and the effects of elastic deformation on the contact patch. It is recognised that adhesion is significant at this scale [20], but is neglected in the current study as a robust model is not yet available but will be implemented in future work. Maw's model characterises the transition between contact patch sliding and sticking using κ , the ratio of the particle's normal and tangential contact stiffness at impact for dissimilar materials (proposed by [21]):

$$\kappa = \frac{\frac{1-\nu_1}{G_1} + \frac{1-\nu_2}{G_2}}{\frac{1-\nu_1/2}{G_1} + \frac{1-\nu_2/2}{G_2}} \quad (2)$$

where subscripts 1 and 2 refer to the particle and substrate respectively. Below a critical impingement angle, Equation 3, the particle slides throughout the period of contact with the wall. However when $\theta_i > \theta_{\text{crit}}$, the particle enters what Maw defines as the intermediate zone where it slides, sticks, then reverts to sliding for most of the remaining contact duration.

$$\theta_{\text{crit}} = 90^\circ - \tan^{-1} (7\kappa - 1) \quad (3)$$

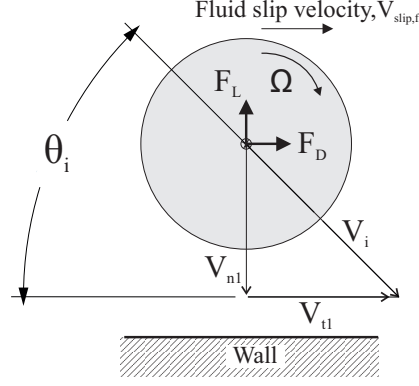


Fig. 1 Particle sign convention.

Between θ_{crit} and 90° , the particle begins to stick progressively earlier during contact. Here, sticking is defined as the local reduction of the particle-wall slip velocity, $V_{slip,w}$ to zero, generating rolling motion. Maw's model is used to develop a low-order model (LoM) for the planar oblique impact of spheres, derived in Section III of this paper. The LoM is subsequently applied to CFD of a simple duct representative of conditions in the secondary-air-system of a gas turbine.

III. Low-Order Model of Tangential Rebound & Rotation

In deriving the rotation model, the particle is assumed to be a sphere impacting a flat, smooth, semi-infinite half-space. It is already known that the angular velocity due to fluid shear is small and that the angular velocity due to particle-wall impacts far upstream will decay due to skin-friction drag, making primary impacts with significant incident angular velocity unlikely. Thus, it is also assumed that the particles do not rotate as they reach the surface. The particle velocities are defined as shown in Figure 1:

$$V_{n1} = V_i \sin(\theta_i) \quad (4)$$

$$V_{t1} = V_i \cos(\theta_i) \quad (5)$$

The average normal force that acts on the particle is calculated by considering the impulse on the particle. Although calculating the actual normal force requires the particle-wall contact time, t_{cont} , as an internal variable it is eliminated during subsequent steps to calculate the CoR_t and particle angular velocity. While an arbitrary t_{cont} is used in the derivation of the model, a non-dimensional contact time $t^* = \frac{t}{t_{cont}}$, $0 < t^* \leq 1$ is employed thereafter. The impulse of the collision $F_{n,ave}^*$ can then be calculated assuming an elastic collision:

$$F_{n,ave}^* = F_{n,ave} t_{cont} = m \Delta V_{n1} \quad (6)$$

$$F_{n,ave}^* \approx 2 m V_{n1} \propto V_{n1} \quad (7)$$

where m is the particle mass. The normal force acting on the contact patch throughout the contact duration is approximated using a sinusoid. The time-dependent normal force can therefore be described by Equation 8:

$$F_n(t^*) = \sqrt{2} F_{n,ave} \sin(t^* \pi), \quad 0 < t^* \leq 1 \quad (8)$$

which is shown in Figure 2a. The instantaneous angular velocity during contact can then be calculated by integrating its angular acceleration:

$$\Omega_{slide}(t^*) = \int \frac{F_n(t^*) \mu r}{I} dt^* \quad (9)$$

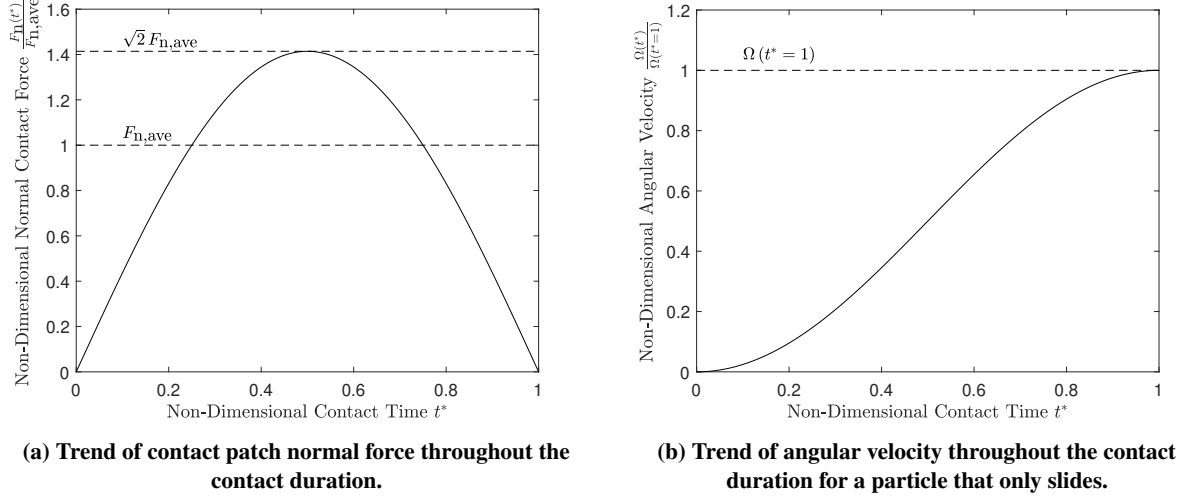


Fig. 2 Trends of representative contact properties.

where μ is the coefficient of friction between the particle and the surface, r is the particle radius and I is the moment of inertia of the sphere. As Equation 9 is a function of Sine through Equation 8, Ω_{slide} should be a function of $-\cos$. Substituting Equation 8 into Equation 9, the constants can be replaced by scaling the Cosine by the - as yet unknown - angular velocity at rebound, Ω , as shown in Figure 2b:

$$\Omega_{\text{slide}}(t^*) = \frac{\Omega(t^* = 1)}{2} [1 - \cos(t^* \pi)], \quad 0 < t^* \leq 1 \quad (10)$$

It is necessary to scale the angular velocity rather than integrate directly from Equation 9 to account for frictional effects described later. It should also be noted that as Ω_{slide} is linearly dependent on normal force, the angular velocity while sliding is also directly proportional to V_{n1} through Equations 7, 8 and 9:

$$\Omega_{\text{slide}}(t^*) \propto F_n(t^*) \propto V_{n1} \quad (11)$$

Once $\theta_i > \theta_{\text{crit}}$, the angular velocity is simply described using rigid body motion:

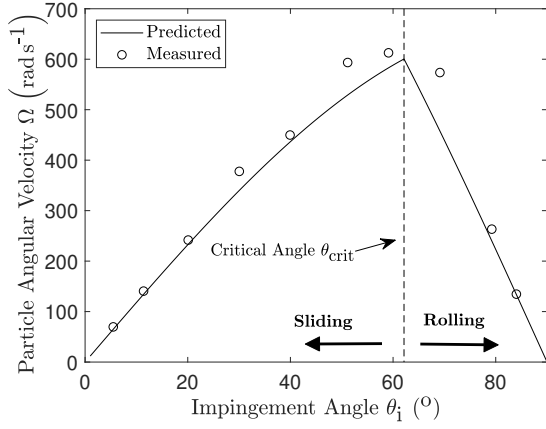
$$\Omega_{\text{roll}} = \frac{V_{t,\text{roll}}}{r} \quad (12)$$

$$V_{t,\text{roll}} = \sqrt{\frac{2(E_{\text{kt1}} - W_{\text{slide}})}{m}} \quad (13)$$

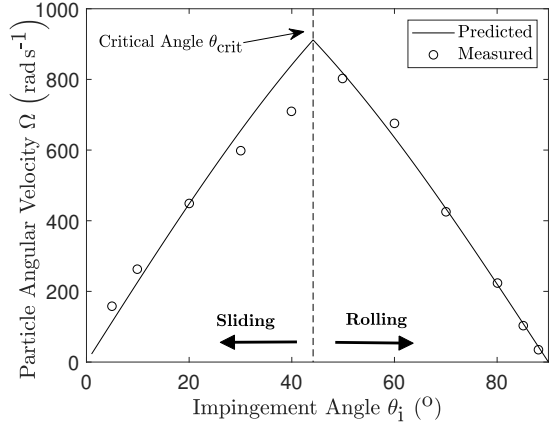
where $V_{t,\text{roll}}$ is the tangential velocity at the point where rolling begins and W_{slide} is the work done by friction between the particle and wall. The incoming tangential kinetic energy of the particle is E_{kt1} . Kinetic energy can only be dissipated through friction when a particle-wall slip velocity exists, i.e. in the sliding regime. As before, the collision is assumed to be elastic. Indeed, even in an inelastic regime it is unlikely that the normal deformation of the contact patch would directly affect the tangential velocity of the particle. The particle-wall slip velocity can be calculated at the critical angle using the average frictional force that acts on the particle and the distance it slides. As, when $\theta_i = \theta_{\text{crit}}$, the slip velocity drops from V_{t1} at $t^* = 1$, to 0 at $t^* = 1$:

$$W_{\text{slide}}(\theta_i = \theta_{\text{crit}}) = \frac{\mu F_{n,\text{ave}}^* V_{t1}}{2} \quad (14)$$

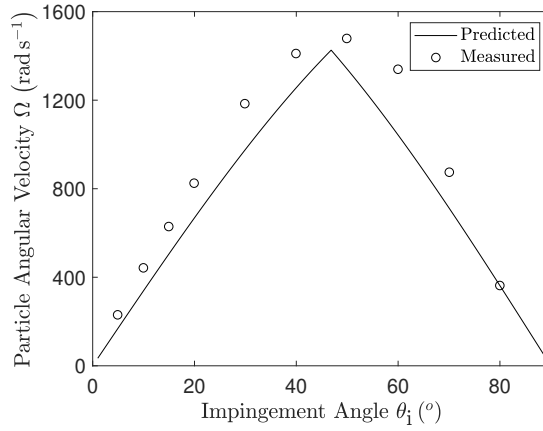
The maximum angular velocity across all impingement angles occurs at $\theta_i = \theta_{\text{crit}}$. At lower impingement angles, the particle only slides as the frictional force is insufficient to cause rigid-body rolling. As θ_i increases the tangential velocity decreases, reducing the angular velocity as shown by Equation 12. The angular velocity below the critical angle will scale linearly with $\sin(\theta_i)$, as shown by Equation 11, while above the critical angle it will scale with $\cos(\theta_i)$ (as shown by Equations 5 and 12). The angular velocity can therefore be scaled by $\sin(\theta_i)$ and $\cos(\theta_i)$ between the fixed points of maximum angular velocity at θ_{crit} and zero angular velocities at $\theta_i = 0^\circ$ and $\theta_i = 90^\circ$:



(a) 5.0 mm Al_2O_3 sphere - glass substrate predictions of angular velocity, compared with data from [22].



(b) 5.0 mm Al_2O_3 sphere - Al2024 substrate predictions of angular velocity, compared with data from [22].



(c) 1.8 mm Al_2O_3 sphere - steel substrate predictions of angular velocity, compared with data from [23].

Fig. 3 Comparison of mm scale Al_2O_3 sphere rebound angular velocity: numerical predictions vs. experimental data.

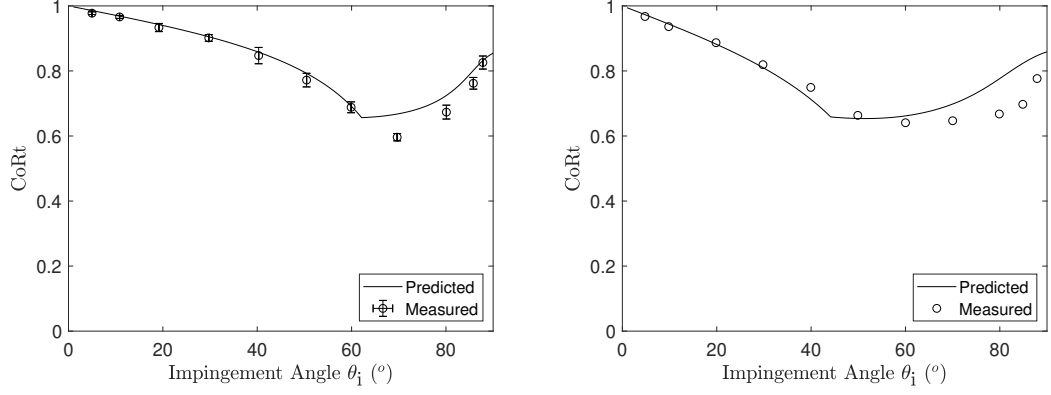
$$\Omega_{\max} = \Omega_{\text{roll}}(\theta_{\text{crit}}) \quad (15)$$

$$\Omega(\theta_i) = \begin{cases} \Omega_{\max} \sin \theta_i / \sin(\theta_{\text{crit}}), & \theta_i < \theta_{\text{crit}} \\ \Omega_{\max}, & \theta_i = \theta_{\text{crit}} \\ \Omega_{\max} \cos \theta_i / \cos(\theta_{\text{crit}}), & \theta_i > \theta_{\text{crit}} \end{cases} \quad (16)$$

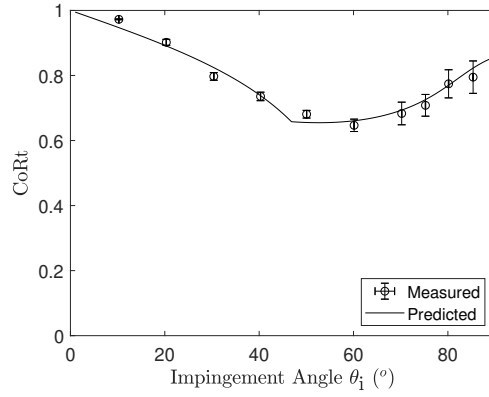
Once the angular velocity at rebound is known, Equation 16, the local angular velocity during the contact duration can be calculated, Equation 10. This then allows CoR_t to be calculated as angular velocity is a key component of both mechanisms that reduce tangential rebound velocity: frictional dissipation and conversion to angular kinetic energy, E_Ω . Frictional dissipation depends on the particle-wall slip velocity $V_{\text{slip},w}$ throughout the contact duration:

$$V_{\text{slip},w}(t^*) = V_t(t^*) - r \Omega_{\text{slide}}(t^*) \quad (17)$$

The work done due to friction is calculated by numerically time-stepping through the contact time, Equation 18:



(a) 5.0 mm Al_2O_3 sphere - glass substrate predictions of CoR_t , compared with data from [22]. (b) 5.0 mm Al_2O_3 sphere - Al2024 substrate predictions of CoR_t , compared with data from [22].



(c) 1.8 mm Al_2O_3 sphere - steel substrate predictions of CoR_t , compared with data from [23].

Fig. 4 Tangential coefficient of restitution of spheres: numerical predictions vs. experimental data.

$$V'_t = \left[\frac{2 \left(\frac{1}{2} m V_t^2 - \mu F_{n,\text{ave}}^* V_{\text{slip},w} dt^* \right)}{m} \right]^{\frac{1}{2}} \quad (18)$$

From the final iteration of Equation 18, the outgoing particle tangential kinetic energy $E_{kt'}$ (considering only frictional losses) can be calculated to approximate the energy dissipated due to friction, E_{wd} . Similarly the tangential rotational kinetic energy at rebound is given by Equation 21:

$$E_{kt'} = \frac{1}{2} m V_t'^2 (t^* = 1) \quad (19)$$

$$E_{wd} = E_{kt1} - E_{kt'} \quad (20)$$

$$E_{\Omega} = \frac{1}{2} I \Omega (\theta_i)^2 \quad (21)$$

When the impingement angle is greater than θ_{crit} , the point in the contact duration where rolling occurs ($V_{\text{slip},w} = 0$) advances as described by Maw et al [16]. It is assumed that it advances from $t^* = 1$ at $\theta_i = \theta_{\text{crit}}$, to $t^* = 0$ at $\theta_i = 90^\circ$, eliminating frictional losses. Therefore, a function $f(\theta_i)$ is included when calculating the outgoing tangential velocity, Equation 22, that reduces linearly from 1 when $\theta_i < \theta_{\text{crit}}$ to 0 at $\theta_i = 90^\circ$:

Table 1 Materials properties used for model validation.

	Sphere	Substrate		
	Al ₂ O ₃	Al2024	Glass	Steel
ν	0.23	0.345	0.25	0.29
G (GPa)	154	26	28	80
μ	-	0.18	0.092	0.163

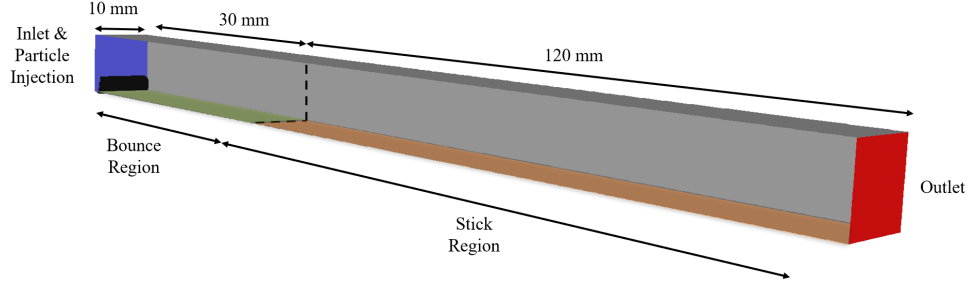


Fig. 5 Computational domain.

$$V_{t2} = \left[\frac{2 (E_{kt1} - f(\theta_i) E_{wd} - E_{\Omega})}{m} \right]^{\frac{1}{2}} \quad (22)$$

This allows the CoR_t to be calculated at a given incidence angle:

$$\text{CoR}_t(\theta_i) = \frac{V_{t2}(\theta_i)}{V_{t1}(\theta_i)} \quad (23)$$

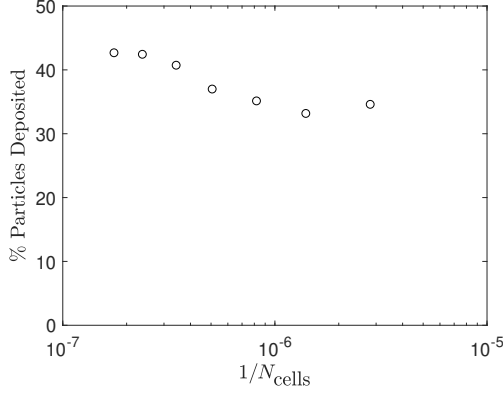
IV. LoM Validation

The model derived in section III was validated by comparison to experimental CoR_t and rebound angular velocity measurements. The data for all validation cases were obtained using alumina spheres of either 5 mm [22] or 1.8 mm [23] diameter with the material properties as shown in Table 1. Adhesive forces have a negligible effect on the experimental data as the particle diameters are much greater than the micron scale [3]; coupon surface roughness is considered small for the same reason. Losses due to stress-wave propagation can be neglected due to the depth of the coupons (these losses are also negligible when compared to plastic deformation [24]). Factors considered by the experimental data are: plastic deformation, elastic deformation and friction.

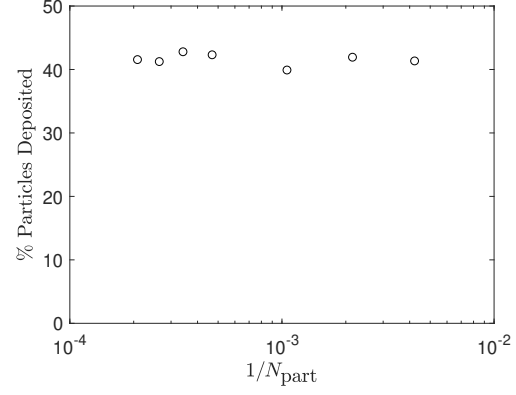
The angular velocities predicted by the model in Equation 16 are shown in Figure 3 where very good agreement is seen with the experimental data from [22] and [23]. The error between numerical predictions and experimental data is an average of 7.8%, 10% and 17% respectively for Figures 3a - 3c. The predictions of CoR_t from Equation 23 are compared with experimental data in Figure 4. General agreement is shown between the model and experimental data with errors of 7.1%, 6.3% and 2.6%. Where differences occur, the location and type are not consistent across all datasets indicating no systemic errors in the model. Error bars are shown where available. The position of the cusp in the CoR_t is not precisely captured and is sharper than in the experimental data, the latter suggesting some spread in experimental results. Overall, the accuracy of the model is considered sufficient when neglecting adhesion.

V. Rotational Particle CFD

The effects of collision-induced rotation on particle trajectories have been examined using ANSYS Fluent 19.2 simulations of a duct that is broadly representative of secondary-air-system geometry using the realisable k- ϵ model



(a) Mesh independence: proportion of injected particles that deposit.



(b) Particle independence: proportion of injected particles that deposit

Fig. 6 Solution independence to mesh and particle injection properties.

with enhanced wall treatment. The duct, shown in Figure 5, has a 10 mm square cross-section and a length of 150 mm. The average inlet velocity is 100 m s^{-1} with a fully-developed boundary layer. Fluid solutions were generated with the outlet set as either atmospheric pressure or 40 barg with fluid densities of 1.23 kg m^{-3} and 19.6 kg m^{-3} respectively. The average inlet velocity was kept constant. Particles are injected downwards at 5° to the streamwise direction and 100 m s^{-1} through an $8 \text{ mm} \times 1 \text{ mm}$ slot at the inlet that is 0.5 mm above the bottom surface of the duct. The Discrete Random Walk model was used for particle tracking with a time scale constant of 0.15.

Particles can escape the domain through the inlet or outlet, are trapped if they collide with the bottom wall in the ‘all-stick’ region $>30 \text{ mm}$ from the entrance and bounce if they collide with any other wall. If they collide with the first 30 mm of the bottom wall - the green ‘all-bounce’ region - the particle rebounds with an angular velocity and CoR_t specified by the model in section III which is implemented as a User Defined Function (UDF). However, where all components of particle velocity are below 0.01 m s^{-1} at impact in the all-bounce region the particle is also assumed to stick. Where the particles bounce, they rebound with a normal coefficient of restitution of unity. All particles are assumed to be subbituminous ash impacting 410 stainless steel with materials properties taken from [3]. Thus the purpose is to investigate the effect of the first bounce on subsequent behaviour rather than generating a fully realistic domain. Simulations are repeated with the angular velocity set to either the predicted value or zero and the resulting deposition compared. The CoR_t predicted by the model in section III is applied in all cases to isolate the effect of rotation. A difference in the number of particles deposited implies that the Magnus force resulting from collision-induced rotation has a significant effect on particle trajectory and deposition in gas turbine components. The OBD model [25] was used to model lift in Fluent as it was most applicable to these particle Reynolds numbers, $Re \approx O(10)$, while the rotational drag acting on the sphere was modelled using [26] which allows particles to acquire angular velocity through fluid shear. As the particles experience significant fluid shear near the wall, the Saffman force is included in all cases in addition to the virtual mass and pressure gradient forces as [27] shows that they become significant near the wall at low Stokes numbers.

A. Mesh Independence Study

Particle deposition is heavily dependent on near-wall flow and therefore mesh density. Atmospheric fluid solutions were produced for a series of similar meshes and particle tracking performed for approximately 4500 $4 \mu\text{m}$ particles with a density of 2077 kg m^{-3} , corresponding to a Stokes number of unity. For mesh sensitivity, the particles were set to rebound with zero angular velocity. Figure 6a shows that particle deposition becomes independent of the mesh with greater than 4×10^6 cells, corresponding to a y^+ uniformly less than unity. This mesh was used in all further simulations.

B. Particle Injection Independence Study

Different numbers of particles of diameter $4 \mu\text{m}$ with a Stokes number of unity were injected into the domain at atmospheric pressure (without collision-induced rotation). Figure 6b shows that the proportion of particles that stuck was independent of the number of particles injected, at approximately 42%. All further simulations therefore inject

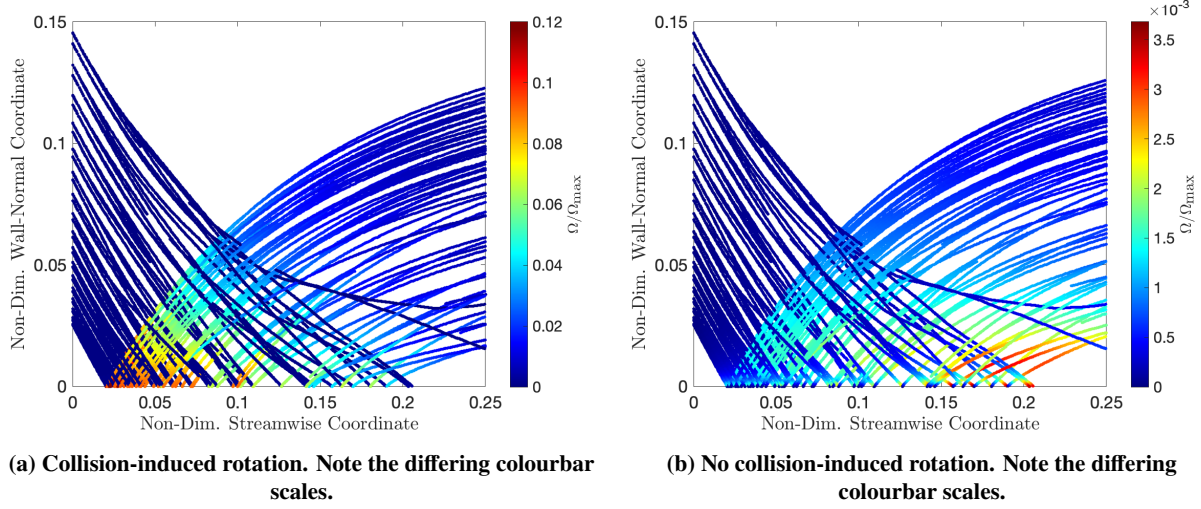


Fig. 7 Atmospheric pressure $6 \mu\text{m}$, $\text{Stk} = 2.5$ particle trajectories showing non-dimensional angular velocity during rebound for a 0.5 mm central slice of the duct. Angular velocities are non-dimensionalised by the maximum possible value for this case Ω_{max} , Equation 25.

approximately 4500 particles for maximum data resolution in cases where a smaller number of particles stick. Were this number of particles to be injected simultaneously in reality, it would increase the local particle-volume fraction beyond the point where one-way coupling is applicable. However, neglecting particle-fluid coupling still allows the relative effect of particle-wall collisions to be established.

VI. Results & Discussion

A series of particle tracking simulations were performed using the atmospheric and 40 barg outlet fluid solutions with both particle diameter and density varied to specify Stokes number, as defined in Equation 24 where μ_g is the dynamic viscosity of the fluid, $\bar{U}_g$ is the bulk velocity and D_h is the hydraulic diameter. All particles enter the domain with zero initial angular velocity and acquire spin through fluid shear or collisions with a wall, as specified by the model in section III.

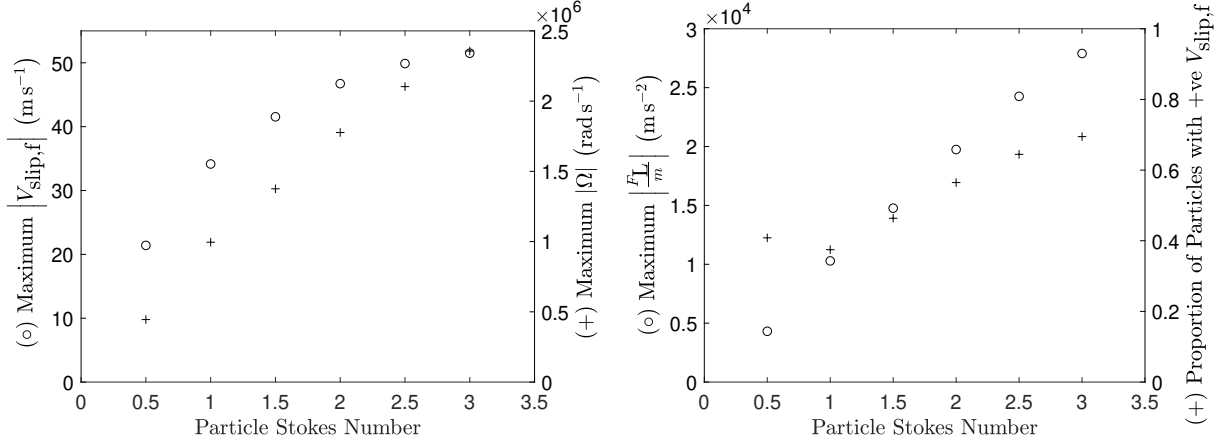
$$\text{Stk} = \frac{\tau_p}{\tau_g} = \frac{\rho_p (2r)^2 \bar{U}_g}{18\mu_g D_h} \quad (24)$$

A. Particle Flow Properties

Figure 7 shows the trajectory coloured by non-dimensional angular velocity of particles impinging on the all-bounce surface, with and without collision-induced rotation enabled. The angular velocities are non-dimensionalised by the maximum possible in this flow, assuming an oblique impact at the flow velocity as shown by Equation 25:

$$\Omega_{\text{max}} = \frac{V_{\infty}}{r} = \frac{100 \text{ m s}^{-1}}{3 \mu\text{m}} \quad (25)$$

where V_{∞} is the free-stream velocity and the particle radius r is that shown for the case in Figure 7. The particles are $6 \mu\text{m}$ in diameter with a Stokes number of 2.5, similar to that of ash particles at atmospheric pressure. It is clear that shear-induced rotation is negligible compared to collision-induced rotation and that rotation persists over a significant path downstream after particle rebound. $V_{\text{slip},f}$ and Ω are the driving components of the Magnus force (Equation 1) and Figure 8 shows the trends of these with increasing Stokes number and the corresponding change in the magnitude of particle wall-normal acceleration. In Figure 8 the maxima are the average of the top 5% of each sample. Despite no dependency of Ω on particle density in section III, the maximum angular velocities increase significantly with Stokes number at a constant particle diameter. This is explained by the increasingly ballistic behaviour of the particles in the boundary layer at higher Stokes numbers, increasing the incidence angle. From Figure 3, higher incidence angles



(a) Trends of maximum $V_{slip,f}$ and Ω magnitudes vs. Stokes number.

(b) Trend of particle wall-normal acceleration and proportion of particles with positive fluid slip velocities.

Fig. 8 Influence of different particle properties on wall-normal acceleration due to the Magnus force at atmospheric pressure. Particles are $6 \mu\text{m}$ and subbituminous ash. Particle density was varied to set Stokes number. Note that F_L was calculated using the correlation from [25].

in the sliding regime increase angular velocity. However, where the particle rolls the opposite is true as also shown by Figure 3. It should also be noted that angular inertia increases with particle density for a given Stokes number, prolonging the period of high angular velocity during rebound and increasing the work done by the wall-normal lift force.

Figures 8a and 9, show that the magnitude of the slip velocity increases with Stokes number and all particles experience regions of positive and negative $V_{slip,f}$. These results agree qualitatively with [13] and suggest that particles may be subject to either positive or negative collision-induced Magnus forces. The behaviour of particles with a Stokes number of 2.5 at atmospheric pressure and 40 barg are also compared in Figure 10. At high pressure the magnitude of the particle-fluid slip velocity is greatly reduced, as the because of the increased drag in the higher density fluid.

The effect of lift due to collision-induced rotation is qualitatively shown by Figure 11 where rebounding particles are accelerated back towards the wall and repeatedly bounce along the surface. Comparing with Figure 9, it is clear that these particles do not escape the region of negative $V_{slip,f}$ near the wall. Particles that escape to a region of positive $V_{slip,f}$, that is being transported by the flow, experience a lift force away from the wall. Overall, there is a bifurcation in particle trajectory: particles that remain close to the wall in a region of negative $V_{slip,f}$ enter a feedback loop that keeps them close to the wall while particles that escape to regions of positive $V_{slip,f}$ are reentrained in the bulk flow.

B. Deposition

The effect of collision-induced rotation on deposition is quantified using the parameter Δr_d , the difference in the percentage of injected particles that deposit with and without collision-induced rotation. Figures 12a and 12b show Δr_d for both the atmospheric and 40 barg outlet cases. A positive Δr_d indicates an increase in deposition with rotation. At atmospheric pressure up to 30% more particles stick with rotation enabled. The position of the peak enhancement of deposition Δr_d increases with particle diameter. Despite Figure 8 showing higher wall-normal acceleration with Stokes number, these increasingly ballistic particles are more likely to escape the region of negative $V_{slip,f}$ in the boundary layer and thus are more likely to be lifted away from the wall, reducing their deposition. This is shown in Figure 8b with the proportion of particles in regions of positive $V_{slip,f}$ increasing with Stokes numbers above one. Below unity, it is expected that slip velocities will progressively tend to zero as $Stk \rightarrow 0$, and hence the proportion of particles experiencing positive $V_{slip,f}$ will tend towards 0.5, as shown for Stokes number = 0.5 in Figure 8b. Therefore, while the magnitude of the lift force becomes more significant with Stokes number, it tends to act to lift particles away from the wall as they become more inertial. However, how this affects deposition will necessarily vary with passage geometry.

Stokes number, Equation 24, is dependent on r^2 . To further investigate the Stokes number distribution under gas-turbine relevant conditions ash particles of varying diameters were tracked with results shown in Figure 12c. At

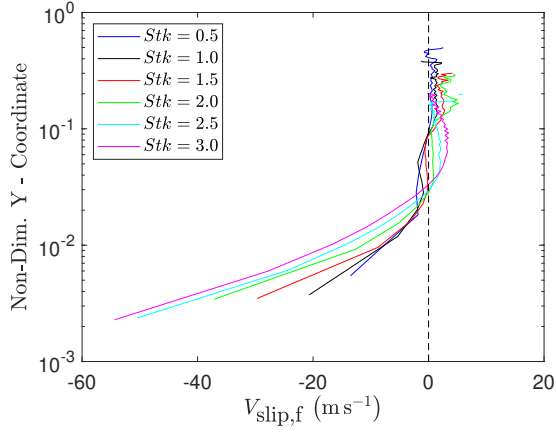


Fig. 9 $6\ \mu\text{m}$ average particle-fluid slip velocities vs. non-dimensional duct height.

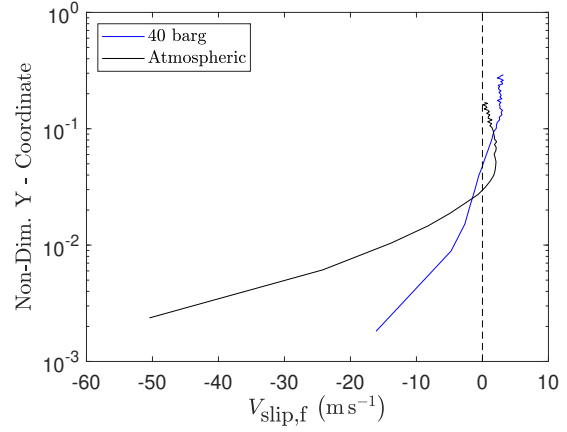
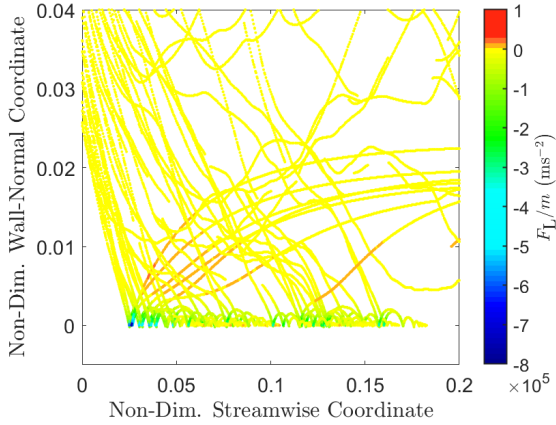
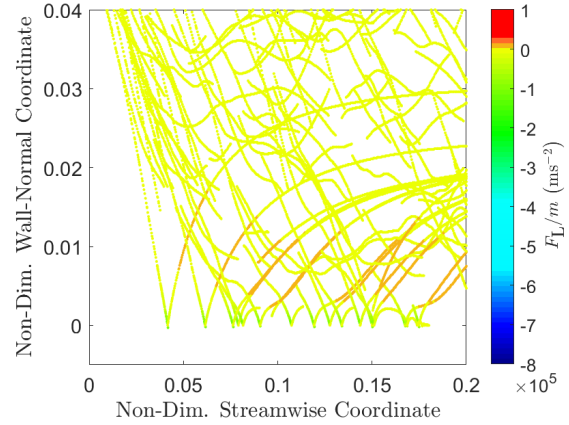


Fig. 10 $6\ \mu\text{m}$ $Stk = 2.5$ particle-fluid slip velocities at atmospheric pressure in atmospheric and 40 barg conditions.



(a) Wall-normal acceleration due to collision-induced lift.



(b) Wall-normal acceleration due to shear-induced lift, no collision-induced rotation.

Fig. 11 $6\ \mu\text{m}$ $Stk = 0.5$ particle trajectories showing wall-normal acceleration due to lift with and without collision-induced rotation for a central $0.5\ \text{mm}$ slice of the duct. The atmospheric flow solution was used. Note that F_L was calculated using the correlation from [25].

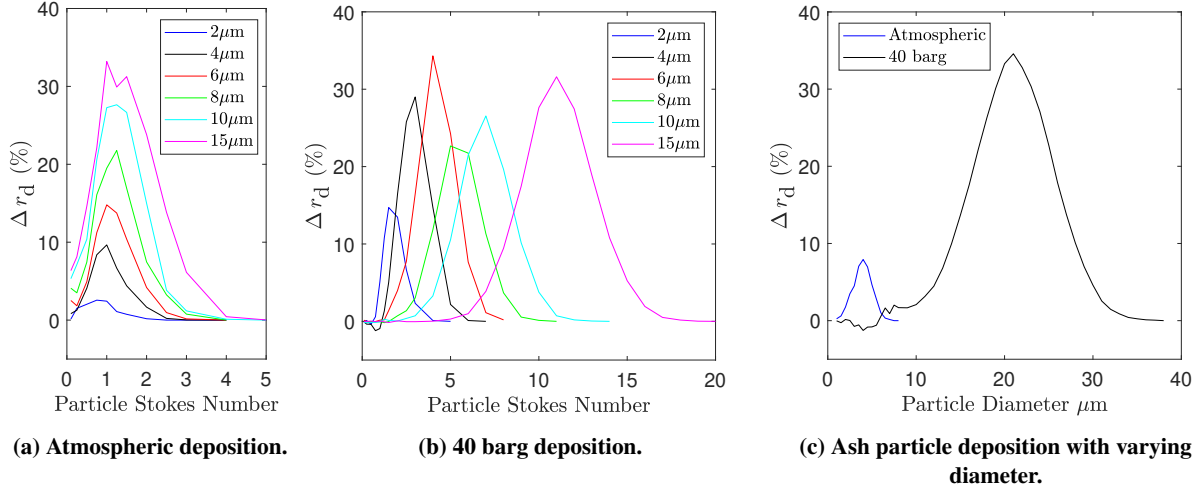


Fig. 12 Increase in deposition with collision-induced rotation.

atmospheric pressure, there was an increase in deposition at diameters between 2 μm and 7 μm . At 40 barg, collision-induced lift has a strong effect on larger particles, resulting in a significant increase in deposition. For example, 35% of 21 μm diameter particles deposit at 40 barg with rotation while none deposit without rotation. This could clearly have a substantial effect on the location and quantity of deposition, underlining the importance of modelling collision-induced rotation in some cases.

VII. Conclusions

The rotation of spheres due to collisions with a wall has been modelled extending well established models used by other workers. Particle rotation is seen to have a significant effect on particle trajectory and deposition under gas-turbine relevant conditions. A model necessary to predict that rotation and the corresponding CoR_t has been presented here and is applicable where van der Waals adhesion is not significant during contact. When modelling the Magnus force, a realistic CoR_t should be applied to produce accurate fluid slip velocities near the wall. The particle Stokes number and diameter are the key parameters that drive particle lift due to their influence on angular velocity and slip velocity. Fluid density was also shown to be an important factor, with the increased pressure of secondary air systems changing the magnitude of lift and the diameter of particles that are affected by rotation. Overall, the effect of collision-induced lift on deposition will vary on a case-to-case basis with geometry, flow-field and particle composition changing how trajectory affects collisions with the wall. In particular, while the magnitude of the lift force increases with Stokes number, in many cases the particles are accelerated away from the wall as they become more inertial. Therefore, the results in Figures 12a - 12c should not be used to state that the effects of collision-induced rotation are insignificant for dissimilar cases without further evaluation. However, it is clear from the results in section VI that collision-induced rotation can have a significant effect on where and how many particles deposit and should be considered when simulating particle transport. Further work will develop a comprehensive bounce-stick model that incorporates adhesion to allow particles at all scales to be modelled accurately.

Acknowledgements

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The statement shall describe the candidate's and co-authors' independent research contributions in the thesis publications. For each publication there should exist a complete statement that is to be filled out and signed by the candidate and supervisor (**only required where there isn't already a statement of contribution within the paper itself**).

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Student Confirmation

Student Name:	Jack Graham Gaskell		
Contribution to the Paper	The research directions employed for the modelling approach, development of analytical models and their implementation in numerical codes, and the majority of the implementation of these codes into a commercial numerical solver were carried out by me as first author. In this role I wrote the manuscript of the paper.		
Signature		Date	23/8/2022

Supervisor Confirmation

By signing the Statement of Authorship, you are certifying that the candidate made a substantial contribution to the publication, and that the description described above is accurate.

Supervisor name and title: David Gillespie, Associate Professor		
Supervisor comments: The motivation for the research was prompted from the overall research aims of the group. Profs. Gillespie and McGilvray supervised the research, identified the overarching research strategy and liaised with Rory Clarkson, who provided industrial oversight from Rolls-Royce the industrial sponsor. Dr. N.Vadgama helped implement the analytical model as a Fluent User Defined Function (UDF).		
Signature		Date 23/8/2022

4 The Rebound of Non-Spherical Particles in Gas Turbine Components

Most current gas turbine particle tracking literature assumes particle sphericity. This greatly simplifies bounce stick modelling, however the sensitivity of particle rebound to the non-sphericity of real particulates was unknown. This paper aimed, primarily, to determine the sensitivity of rebound to non-sphericity and, secondly, to understand how the collision physics differed from the spherical case. Finite element simulations demonstrated that rebound is highly sensitive to sphericity and hence should be included in bounce stick models. Three primary differences were identified between spherical and non-spherical collision physics:

1. The horizontal displacement between the contact patch and particle centre of mass results in an additional moment about the particle centroid;
2. The contact patch geometry varies with particle orientation, being ‘sharper’ when impacting end-down;
3. The particle may collide with the wall multiple times per collision event, resulting in the transfer between linear and angular forms of kinetic energy.

A fourth finding identified the so-called “self-servo” effect, where particle rotation would alter the wall-normal pressure and hence friction. These findings showed that a force-based approach was best suited to model non-spherical particles, hence guided the selection and design of a DEM-based method for the bounce stick model described in the next chapter. It also demonstrated the importance of their inclusion in rebound modelling, justifying the investment in the development and validation of a non-spherical model. Finally, it provided a dataset to validate the predictions of the collision model in Chapter 5. The paper was originally presented by the author of this thesis at the 14th European Turbomachinery Conference (ETC14). All material presented was produced by the same author, with Professors Gillespie and McGilvray supervising the research.

THE REBOUND OF NON-SPHERICAL PARTICLES IN GAS TURBINE COMPONENTS

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ABSTRACT

Particulate deposition can cause significant damage to gas turbine components. Modelling the location and quantity of deposition is desirable to optimise component geometry and quantify cost of ownership effects that arise from the ingestion of atmospheric contaminants. Bounce-stick modelling predicts whether a particle will bounce, stick or shatter upon impact with a wall. Current modelling assumes that particles are spherical, which is not the case for real atmospheric particulates. This paper uses FEA to examine the sensitivity of particle rebound trajectories to non-sphericity and characterise the collision physics of spheroids. Rebound trajectories are shown to differ significantly from those of equivalent spheres with a strong dependence on particle orientation. Significant angular velocities are observed upon rebound, which vary in both sign and magnitude with the potential to affect downstream trajectories through the Magnus force. Future bounce-stick models should include the effects of non-sphericity to accurately predict rebound trajectories and downstream deposition.

KEYWORDS

Particles, Bounce-Stick, Gas Turbines, Deposition, Sand.

NOMENCLATURE

τ_p^+ Non-dimensional particle relaxation time from Marchioli et al., 2010

$\text{CoR}_n, \text{CoR}_t$ Normal and tangential coefficients of restitution, $|V_{n2}/V_{n1}|$ and V_{t2}/V_{t1}

θ_i, θ Particle impingement and orientation angles, $^\circ$

θ_x Component of particle orientation angle θ from Marchioli et al., 2010

A_{proj} Particle maximum projected area, m^2

D_p Particle equivalent spherical diameter, m

L_{proj} Particle maximum projected length, m

$M_{\text{fric}}, M_{\text{rebound}}$ Particle centroid moments due to friction and non-spherical geometry, Nm

P Particle perimeter, m

V_i, V_{n1} & V_{t1} Particle initial total, normal and tangential velocities, ms^{-1}

y^+ Dimensionless wall distance, defined by friction velocity (Marchioli et al., 2010)

AR, Sh Particle Aspect Ratio and Shape Factor

INTRODUCTION

Ingested atmospheric particulates are known to cause significant damage to gas turbine components, notably through deposition in the secondary air system and turbine blade cooling passages (Dunn, 2012). The reduction in flow capacity and corrosion that often results are a major driver of in-service maintenance costs and loss of cooling effectiveness. The ability to accurately model deposition would enable the design of more durable components and better predictions of maintenance requirements.

Bounce-stick models are used to determine whether a particle bounces, sticks or shatters upon impact with a wall. They may also predict the trajectory of rebound by providing values of coefficient of restitution (CoR), the ratio of outbound to inbound linear velocity components. Where a sphere collides with a smooth substrate, the impact is assumed to be as defined in Figure 1. Existing bounce-stick models, notably (Bons et al., 2017; Yu and Tafti, 2019; Brach and Dunn, 1992) assume that particles are cylindrical or spherical to reduce the mathematical complexity of their approaches. However, there is little published literature on the sensitivity of particle rebound to non-sphericity typical of real ingested particulates. A simple soft-sphere type approach was used by Wynn (2009) to model the rebound of spheroids, finding that multiple bounces may occur and that rebound becomes more distinct from that of a sphere with increasing non-sphericity. Stochastic corrections for non-sphericity have also been developed (Whitaker and Bons, 2018), however they are necessarily limited to the specific particle shapes, sizes and materials tested without modelling the underlying collision physics.

Reid (2003) describes the composition and morphology of atmospheric contaminants sampled between ground level and 5000 m altitude. The dust was collected over Puerto Rico having originated in Africa, the world's largest source of mineral dust (Chou et al., 2008). Particle morphology did not vary significantly with altitude and all particles were characterised as prolate spheroids using two primary parameters: aspect ratio (AR) and shape factor (Sh) as described in Equations 1 and 2:

$$AR = \frac{\pi L_{\text{proj}}^2}{4A_{\text{proj}}} \quad (1)$$

$$Sh = \frac{P^2}{4\pi A_{\text{proj}}} \quad (2)$$

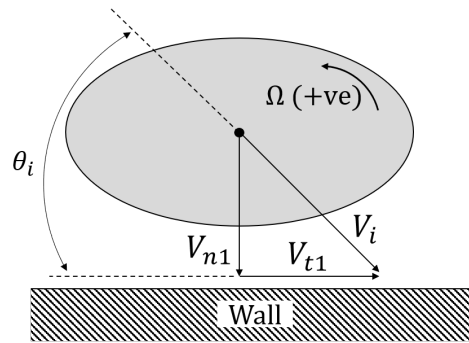


Figure 1: Particle sign convention

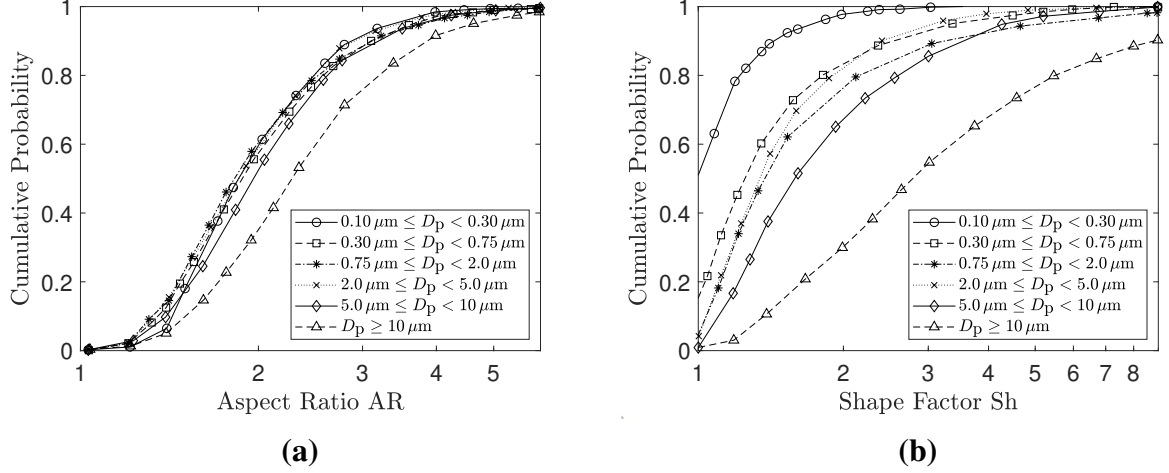
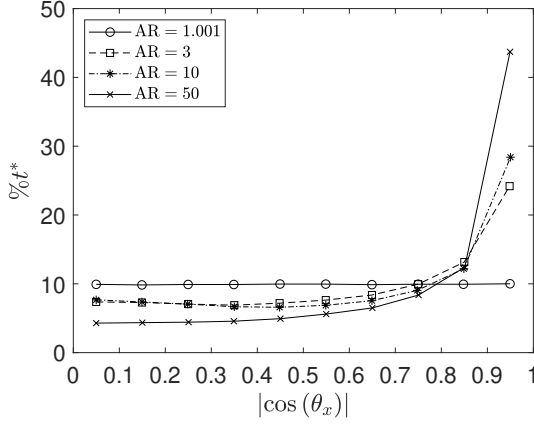


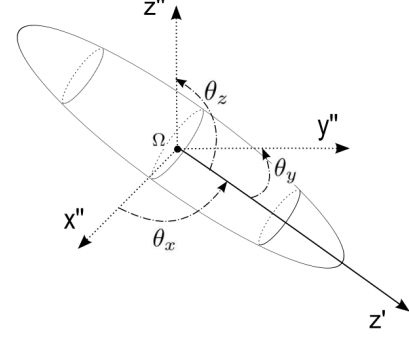
Figure 2: Airborne particulate morphology from Reid (2003)

Approximating the shape of real particulates as prolate spheroids, the Aspect Ratio (AR) is the best fit ratio of major to minor axis lengths while shape factor is a measure of particle roundness where values greater than unity describe a more “jagged” shape. Aspect ratio did not vary significantly with particle diameter with a median value of 1.9 and standard deviation of 0.9 as shown in Figure 2a, similar to the values reported in (Chou et al., 2008). Particle shape factor did vary significantly with size, as shown by Figure 2b. Higher particle surface roughness will likely increase plastic deformation and lower the normal coefficient of restitution. However, to study the bulk effects of non-sphericity only the effects of aspect ratio will be considered in the present work.

Previous workers have shown through DNS that non-spherical particles behave differently in near-wall turbulence when compared to spheres. The wall-normal velocities of inertial elongated fibres, studied by Marchioli et al. (2010), are affected by both aspect ratio and inertia. Non-monotonic variations of wall-normal velocity are observed with changing AR and particle relaxation time τ_p^+ . This behaviour is explained by the rate at which the particles are centrifuged out of near-wall vortex cores due to inertia and attain different positions on the vortex periphery based on their elongation, thus “seeing” different local flowfields. This effect is shown by a greater relative concentration of higher aspect ratio particles near the wall. This translates into a greater likelihood of higher aspect ratio particles colliding with the wall across all values of τ_p^+ considered. Marchioli et al. (2010) also studied the preferential orientation of spheroids near the wall, finding that spheroids with a higher aspect ratio were more likely to orient their long axes with the mean streamwise direction in turbulent channel flow, as shown by Figure 3. This implies that real particles are more likely to “tumble” end-over-end when colliding with the wall, rather than to “log-roll”. This matches the findings of Jie et al. (2019) who also propose an explanation for the phenomenon, related to fluid Lagrangian stretching and compression. Therefore, it is known that anisotropic particles are more likely to collide with a wall than their spherical equivalents and that they are more likely than not to collide while tumbling: the manner most distinct from spheres. This configuration is used in the present work, with the spheroids’ major axis and velocity vectors in the plane normal to the wall.



(a) $\tau_p^+ = 1$



(b) Particle orientation sign convention, x'' is the mean streamwise direction

Figure 3: From Marchioli et al. (2010). Percentage of time that particles spend with a given orientation, where dimensionless wall distance $y^+ < 10$

Where a particle rebounds from a surface, bounce-stick models predict the outbound trajectory. Where multiple bounces occur, the effect of collisions on downstream trajectory will determine where or if deposition occurs. The angular velocity and position in the boundary layer of rebounding micron-scale particulates was shown by Gaskell et al. (2020) to significantly affect the trajectory of rebounding spheres through the Magnus force: CFD of a secondary air system-representative duct showed instances of up to 35% of injected particulates depositing with collision-induced rotation (CIR) while none deposited where the CIR model was disabled. Therefore, deviations in particle angular velocity and trajectory due to non-sphericity could significantly affect the likelihood of subsequent wall collisions.

The present work aims to determine the sensitivity of particle rebound trajectory to non-sphericity, considering geometries relevant to the particles ingested by gas-turbines. It also aims to describe how the collision dynamics of spheroids differ from those of spheres to aid in the development of bounce-stick models that capture particle non-sphericity.

METHOD

Airborne particulates can be characterised as prolate spheroids defined by an aspect ratio, Equation 1. Here, ANSYS Mechanical 19.2 is used to simulate the collision between alumina particles and a flat plate. Two angles characterise the configuration of the spheroid: the impingement angle θ_i and the orientation angle θ . The impingement angle is defined as in Figure 1 and denotes the angle of the particle's incoming velocity vector relative to the surface. The orientation angle describes the offset between the spheroid's long axis and the ground plane, defined where the ground plane is line $\overline{AB}$ in Figure 4a. Orientation angle is defined as negative to keep with a counterclockwise-positive sign convention in Figure 4a. The rebound of a prolate spheroid with $AR = 1.9$, the average value from Reid (2003) for airborne particulates near ground level, is compared with a sphere of equivalent volume. Two different particle incidence angles are considered, $\theta_i = 5^\circ$ and $\theta_i = 45^\circ$ with a range of particle orientation angles, between $\theta = 0^\circ$ and $\theta = -180^\circ$. Airborne particulates at the compression system exit of gas turbines have

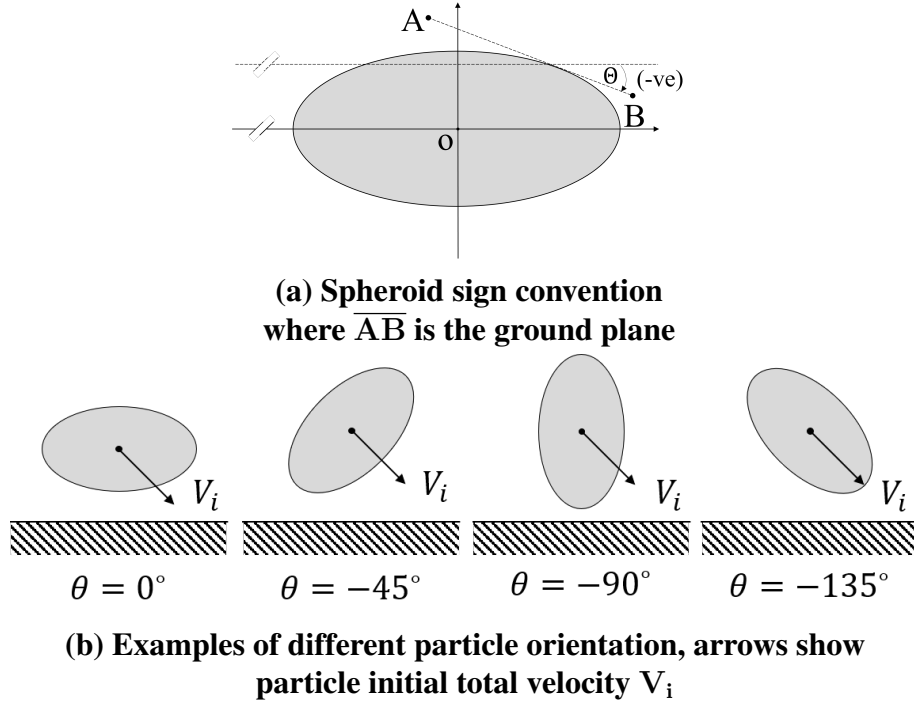


Figure 4: Particle orientation sign convention

an average diameter of $6 \mu\text{m}$ (Clarkson et al., 2016) with a range of material compositions, however millimetre-scale particles are studied here to enable validation against experimental data from (Gorham and Kharaz, 2000). This also decouples adhesive effects from spheroidal collision dynamics as particles much greater than $10 \mu\text{m}$ in diameter do not experience strong adhesive effects (Whitaker and Bons, 2018).

The alumina particles have an equivalent spherical diameter of 5 mm and collide with an Al2024 substrate at $V_i = 3.9 \text{ ms}^{-1}$ to match the experimental setup of Gorham and Kharaz (2000). The impact of equivalent spheres is compared with experimental data for validation, with the same computational setup extended to spheroids. Half-plane symmetry was applied to reduce compu-

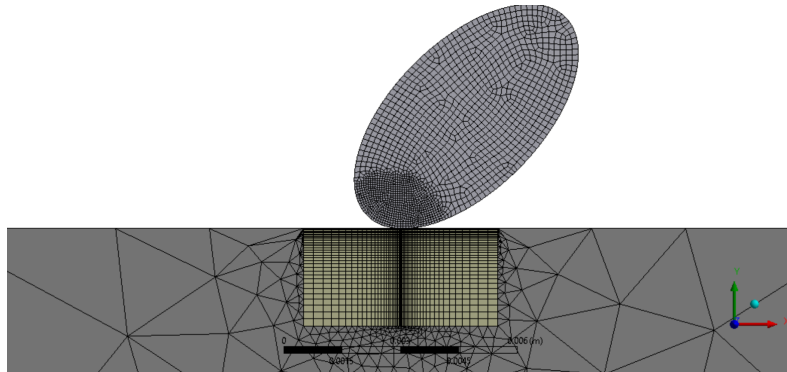


Figure 5: Mesh of $AR = 1.9$ spheroid at $\theta = -45^\circ$ with 2.75×10^5 elements

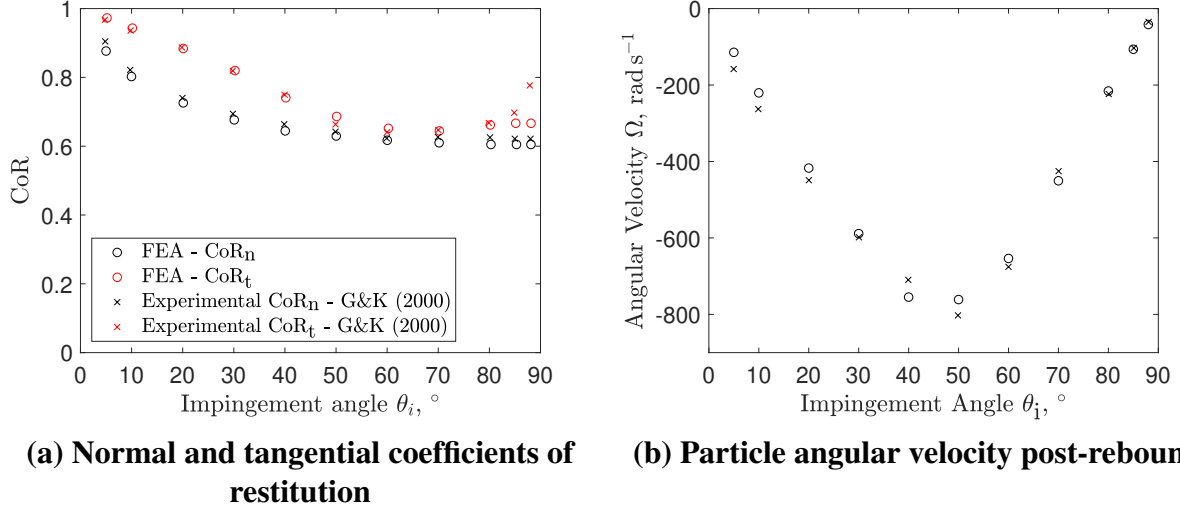


Figure 6: FEA simulations of $\varnothing 5$ mm alumina spheres ($\circ$) at a range of impingement angles compared to experimental data ($\times$) from Gorham and Kharaz (2000)

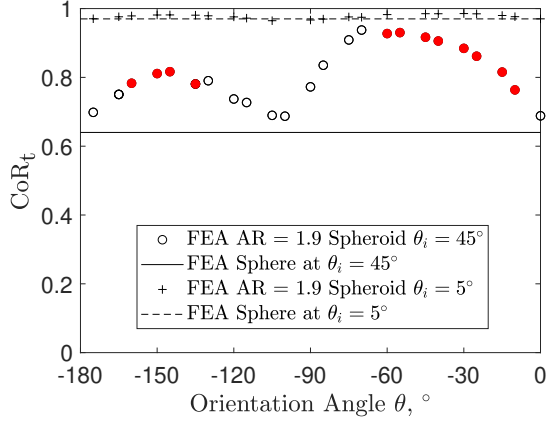
tational time with local mesh refinement at the point of impact for both the particle and substrate. The substrate is a coupon that, without symmetry, measures $140 \text{ mm} \times 140 \text{ mm} \times 25 \text{ mm}$. Hex-dominant meshing is used throughout the particle and contact region of the substrate to reduce cell count, while a tetrahedral mesh is used for the larger cells that comprise the remainder of the coupon, as shown by the contact point geometry in Figure 5.

Mesh Independence & Validation Study

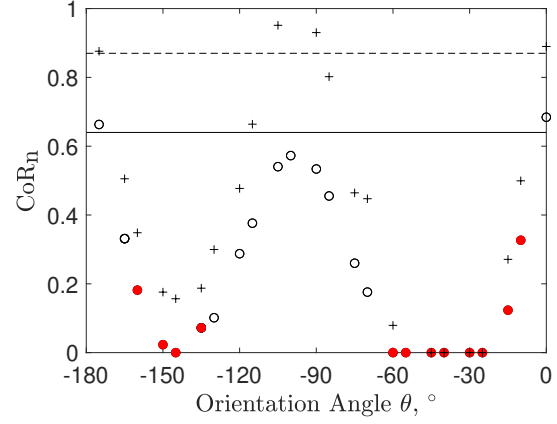
FEA simulations were performed of 5 mm diameter spheres colliding with the substrate at $\theta_i = 50^\circ$, matching an experimental value that was close to the mid-point between a normal and oblique collision and hence allowing comparisons between FEA and experimental data. Simulations were performed with different meshes to ensure solution independence from element size. The ratios between the sizes of elements in different regions were kept constant with the total number of elements varied between 1.55×10^5 and 5.14×10^5 . A mesh with 2.78×10^5 elements was the most computationally efficient with a runtime of five hours across ten cores. Deviations of only 0.7%, 1% and 1% were recorded between the 5.14×10^5 element and 2.78×10^5 meshes for CoR_n, CoR_t and Ω respectively. This number of elements or greater, with the same element size at the contact patch, was used for all subsequent simulations. Further comparison with experimental data from Gorham and Kharaz (2000) is shown in Figure 6 with good agreement between FEA and experiments. Overall, FEA is shown to accurately represent collisions of millimetre-scale particles.

RESULTS

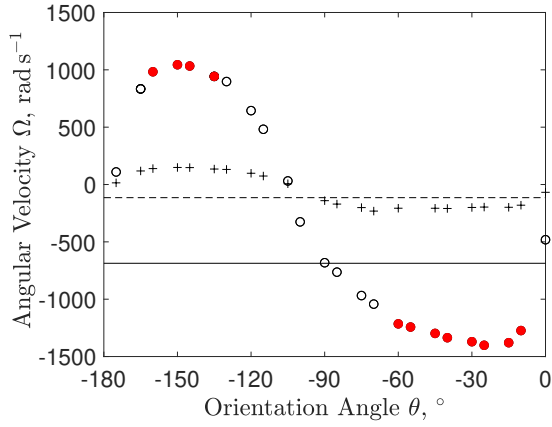
The primary and secondary impacts of AR = 1.9 spheroids were simulated in FEA. For primary impacts, collisions were simulated at $\theta_i = 5^\circ$ and $\theta_i = 45^\circ$. Simulations of secondary collisions, where the particle re-collides with the wall shortly after the first impact, were performed using rebound trajectories from primary collisions where $\theta_i = 45^\circ$. In all cases, rebound was defined as the point at which contact surface pressure returned to zero, indicating the particle was no longer in contact with the substrate.



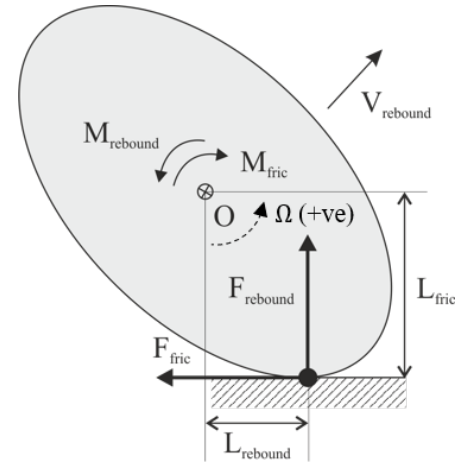
(a) Tangential coefficient of restitution



(b) Normal coefficient of restitution



(c) Particle angular velocity post-rebound



(d) Schematic of spheroid rebound at $\theta = -135^\circ$

Figure 7: The rebound of AR = 1.9 spheroids following primary collisions at a range of orientation angles, θ_i is 45° or 5° . Red data points indicate a second collision occurs

Primary Collisions

The rebound properties of the AR = 1.9 spheroid at different orientation angles relative to the surface are shown in Figure 7. All values are taken at the point of rebound following the first bounce, so do not show the effect of multiple bounces occurring as described in the following subsection. Where a secondary collision occurs, the primary impact is highlighted red.

The collision kinematics of a prolate spheroid are shown schematically in Figure 7d. Both a sphere and a spheroid experience a moment about their centroids due to friction with the surface and their tangential velocity, M_{fric} . However, as the line of action of rebound will not always act through the spheroid centroid, a spheroid will experience an additional moment, M_{rebound} . This moment depends entirely on the normal component of impulse as F_{rebound} is always normal to the wall and hence couples CoR_n and Ω . This is shown by comparing the maxima and minima from Figures 7b and 7c. This leads to a significant increase in the magnitude of angular velocity where the sign varies depending on the orientation angle,

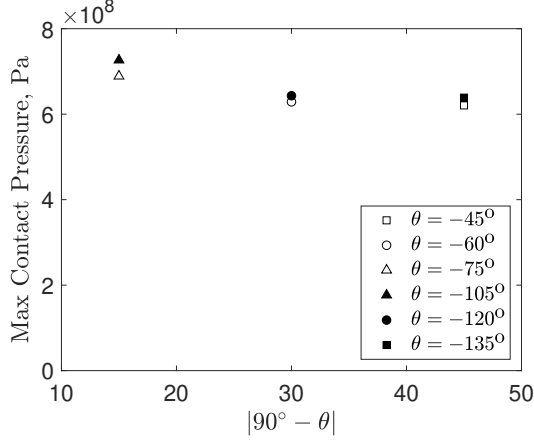


Figure 8: Contact patch maximum surface pressure for collision pairs symmetrical about $\theta = 90^\circ$ for a collision where $\theta_i = 45^\circ$

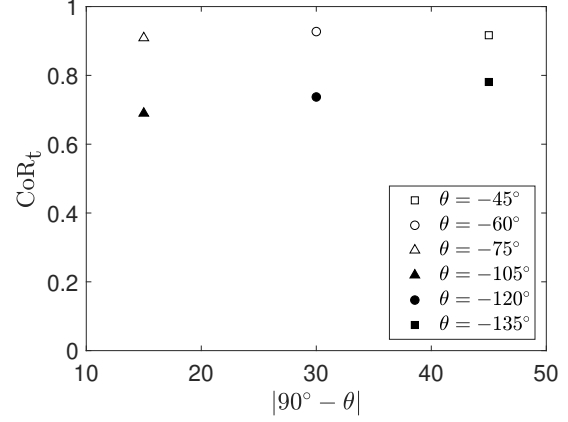


Figure 9: Tangential coefficient of restitution for collision pairs symmetrical about $\theta = 90^\circ$ for a collision where $\theta_i = 45^\circ$

rotating both clockwise and anti-clockwise where an equivalent sphere rotates only clockwise. In Figure 7d, M_{rebound} opposes M_{fric} however where $-90^\circ < \theta < 0$ they will act in the same direction. This explains the greater magnitude of the angular velocities where $\theta > -90^\circ$ in Figure 7c. Figure 7b also shows that there is almost always a decrease in CoR_n compared to the equivalent spherical case. Where $\text{CoR}_n = 0$, the direction of the spheroid centroid velocity is still towards the wall following the first collision as the centroid pivots around the contact patch. The reduction in CoR_n will increase the time spent by the particle in the surface boundary layer. Combined with the increased magnitude and changing sign of Ω , and the trend of increasing CoR_t above the equivalent spherical value, discussed later, the rebound trajectory of a spheroid is more susceptible to the influence of the Magnus force as described by Gaskell et al. (2020).

The contributive or opposing moments also explain the smaller peak of CoR_t in Figure 7a where $-180^\circ < \theta < -90^\circ$, as M_{fric} acts to increase surface pressure and hence friction. This is analogous to the “self-servo” effect observed in drum brakes. Conversely, where $-90^\circ < \theta < 0$, M_{fric} acts to lift the contact patch away from the surface. This is shown by Figures 8 and 9 where geometrically similar collisions with the same angular displacement from $\theta = 90^\circ$, e.g. 85° and 95° , have higher maximum surface pressures where $\theta < -90^\circ$. Geometrically similar means, here, that the local surface curvature at the point of contact is the same and the centroid has the same vertical displacement from the collision surface. As friction is the only factor to influence CoR_t , higher surface pressures increase tangential losses.

The locations and magnitude of the CoR_t maxima in Figure 7a are also explained by Figure 7b through impulse: maximum average normal force will occur when $\text{CoR}_n = 1$. Reductions in CoR_n will reduce the average normal force at the contact patch and hence tangential friction. Similar trends can be seen when $\theta_i = 5^\circ$ where the CoR_t ranges between the equivalent spherical value and unity, inversely correlating with the drop in CoR_n . Spheroid collisions normalised by the equivalent spherical values are shown in Figure 10 for CoR_n and Ω , where the closeness of fit between impingement angles indicates that the underlying collision physics are similar for

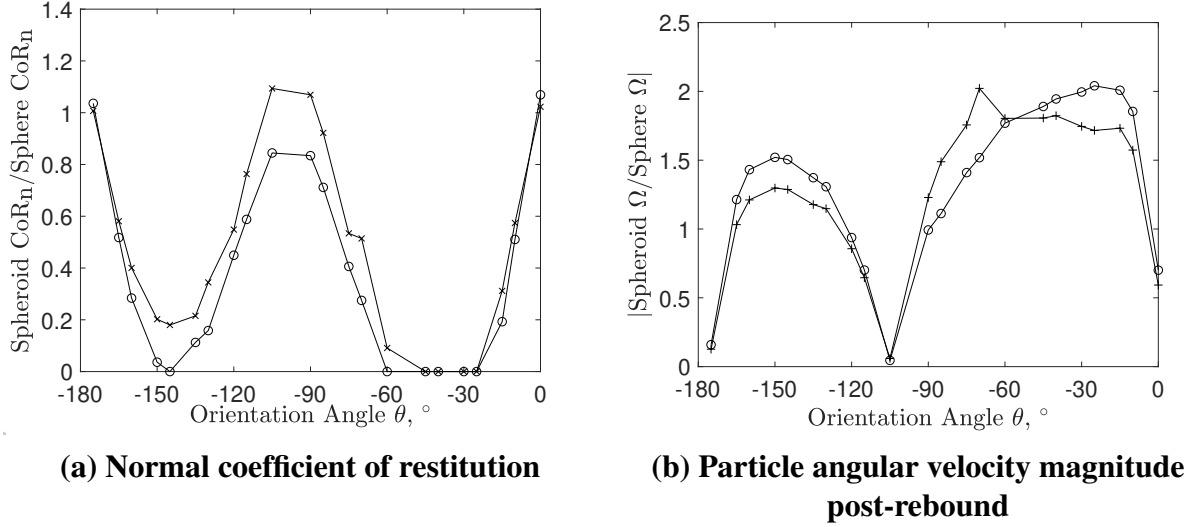


Figure 10: The rebound properties of AR = 1.9 spheroids following their primary collisions where $\theta_i = 5^\circ$ and $\theta_i = 45^\circ$, normalised by the value for an equivalent sphere

both cases.

Following a primary collision, the rebound of spheroids vary significantly from the rebound of spheres. Tangential coefficient of restitution varies between the equivalent spherical value and unity, with average and maximum increases of 20% and 50% for the $\theta = 45^\circ$ cases, excluding cases where second bounces occur. CoR_n is lower than the equivalent spherical value with a maximum decrease of 84%. Linear kinetic energy is transferred to angular kinetic energy, resulting in angular velocities up to twice as large as those of spheres and often rotating in the opposite direction. Collision physics for normal rebound and angular velocity appear similar for different impingement angles, when normalised by the equivalent spherical value.

Secondary Collisions

Directly simulating multiple collisions in FEA is impractical due to the computational time required and the need for mesh refinement at each point of impact. It is also unnecessary in order to capture secondary collisions occurring immediately following the primary collision. For these collisions, additional external forces are not required, and indeed they modify the particle trajectory insignificantly in the time period considered. Therefore they are not modelled. The FEA models the collision until the point of detachment from the model surface. For a secondary collision to occur it is only necessary that the particle rotation about its centroid is sufficient to bring a point on the ellipsoid surface back into contact with the underlying substrate. The likelihood of this changes with changing rotational speed, aspect ratio, initial impact position and velocity vector leaving the surface. Therefore, the normal, tangential and angular velocities of the spheroids following the first bounce are held constant and an explicit time-stepping scheme implemented in Matlab used to predict whether secondary collisions would occur, and at what orientation angle, θ . Secondary impacts were simulated using FEA data from impacts where $\theta_i = 45^\circ$. The plane on which the particle major axis lies is always aligned normal to the wall in these cases, thus modelling the trajectory of the particle cross-section (ellipse) is sufficient to determine exactly the position of secondary impact, where the particle is translated linearly

Table 1: Orientation of particles at the point of secondary impact

Primary θ °	-10.0	-15.0	-25.0	-30.0	-40.0	-45.0	-55.0	-60.0	-135	-145	-150	-160
Secondary θ °	-147	-158	-163	-162	-158	-153	-138	-124	-60.6	-34.2	-32.2	-39.4

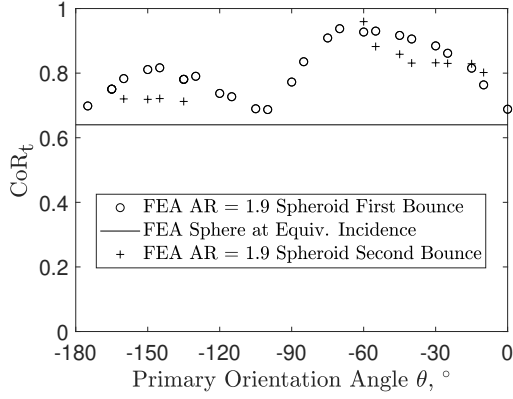
and rotated about its centroid as per the rebound velocity vectors from its primary collision. The model commences at the point of rebound and continues to displace the 2D representation of the ellipsoid until either it re-collides with the ground plane or is sufficiently far from the surface that it will not re-collide. This allows predictions of whether a secondary bounce will occur in addition to providing the particle orientation at the point of re-collision. A timestep sensitivity study confirmed that $\mathcal{O}(10^3)$ timesteps adequately resolved particle motion. The results of this model are shown in Table 1 using inputs from Figure 7, with only those that re-impacted the wall shown. New FEA simulations were performed with the rebound angular, normal and tangential velocities shown in Figure 7 using the orientation angles in Table 1. The same computational setup as as first bounce simulations was used with results shown in Figure 11. Note that the coefficients of restitution and orientation angles shown are with respect to particle velocities and orientation prior to the first collision.

Particles experience a transfer between linear and angular kinetic energies during their primary collisions, as explained previously. From Figures 11b and 11c, this linear kinetic energy is recovered during a secondary collision with the magnitude of angular velocities following the second rebound smaller than the equivalent spherical value and that of the primary rebound. This results in a higher CoR_n than a first collision alone. Therefore, the magnitude of angular velocity may be between 52% greater ($\theta = -70^\circ$) and 95% lower ($\theta = -105^\circ$) than an equivalent sphere when considering first and second bounces. If all linear kinetic energy transferred to angular kinetic energy is recovered, it might be expected that the angular velocity would be the same as the spherical value given that only friction would influence Ω , as for a sphere. However, as angular velocity due to friction is derived from tangential impulse, increased CoR_t implies reduced friction and hence explains the lower angular velocities compared to an equivalent sphere.

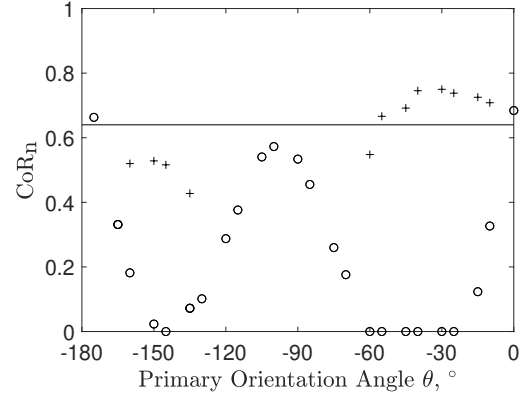
Where secondary bounces occur, angular kinetic energy derived from the normal impulse of the first collision will be recovered and lead to a CoR_n similar to that of a sphere. Contact patch friction and therefore CoR_t is largely unaffected by incoming angular velocity and hence is similar to that of a primary impact. The magnitude of angular velocity following a secondary collision is lower than the equivalent spherical value and that of a primary collision. The greatest overall reduction of CoR_n in combined primary and secondary collisions is 84% at $\theta = -130^\circ$. Analysis of the second bounce FEA simulations showed that no tertiary collisions occurred.

CONCLUSIONS

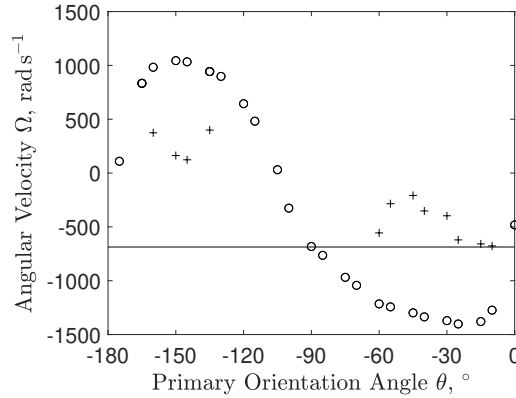
The rebound of a spheroid with $\text{AR} = 1.9$, broadly representative of an atmospheric particulate that may enter a gas turbine, varies significantly from that of an equivalent sphere. Considering the combined first and second bounces, the CoR_n may be up to 84% lower than the equivalent spherical value while the CoR_t may be up to 50% greater. The trajectory following both pri-



(a) Tangential coefficient of restitution



(b) Normal coefficient of restitution



(c) Rebound angular velocity magnitude

Figure 11: Rebound properties of AR = 1.9 spheroids during primary and combined primary-secondary collisions. $\theta_i = 45^\circ$ prior to the first collision

primary and secondary impacts will have a CoR_t higher than the equivalent spherical value but below unity, as unlike the coupling between CoR_n and Ω , tangential impulse is only affected by friction. If only one impact with the wall occurs, the normal velocity of the particle during rebound is likely to be significantly lower than that of an equivalent sphere while the occurrence of a second impact recovers angular kinetic energy and leads to a CoR_n similar to an equivalent sphere. Particle angular velocity following any number of impacts is likely to be affected by non-sphericity, changing sign with a magnitude between 152% and 5% of the equivalent spherical value. This affects particle trajectory and the likelihood of subsequent deposition through the Magnus force. Normalisation of the results showed no fundamental differences between the collision dynamics of particles at different impingement angles. This suggests a means by which a surrogate model for non sphericity might be implemented in the future.

The normal and tangential aspects of spheroidal collision dynamics are highly coupled, presenting challenges when developing bounce-stick models for non-spherical particles. Whether particles re-collide immediately with the surface was found using a simple time-stepping scheme. Indeed, predicting whether a second bounce occurs and its effects are crucial to accurately predicting particle downstream trajectory. The results presented here provide a sensitivity analysis

of particle rebound to non-sphericity and can also be used as validation data for future bounce-stick models. The rebound trajectories shown here demonstrate that particle non-sphericity must be considered in bounce-stick models to accurately predict downstream deposition.

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Statement of Authorship for joint/multi-authored papers for PGR thesis

To appear at the end of each thesis chapter submitted as an article/paper

The statement shall describe the candidate's and co-authors' independent research contributions in the thesis publications. For each publication there should exist a complete statement that is to be filled out and signed by the candidate and supervisor (**only required where there isn't already a statement of contribution within the paper itself**).

Title of Paper	The Rebound of Non-Spherical Particles in Gas Turbine Components
Publication Status	☒ Published ☐ Accepted for Publication ☐ Submitted for Publication ☐ Unpublished and unsubmitted work written in a manuscript style
Publication Details	Gaskell, J. G., McGilvray, M., Gillespie, D. R. H. (2021a). "The Rebound of Non-Spherical Particles in Gas Turbine Components." Proceedings of 14th European Conference on Turbomachinery Fluid Dynamics & Thermodynamics. Virtual, Online. April 12-16, 2020. https://doi.org/10.29008/ETC2021-653

Student Confirmation

Student Name:	Jack Graham Gaskell		
Contribution to the Paper	As first author, I specified the research strategy including the number of simulations and their design. For example, determining what geometries to examine from literature, modelling them, then setting up and running the FEA software. I post-processed all the results and wrote the manuscript of the paper.		
Signature		Date	23/8/2022

Supervisor Confirmation

By signing the Statement of Authorship, you are certifying that the candidate made a substantial contribution to the publication, and that the description described above is accurate.

Supervisor name and title: David Gillespie, Associate Professor			
Supervisor comments: The motivation for the research was prompted from the overall research aims of the group. Profs. Gillespie and McGilvray supervised the research and identified the overarching research strategy.			
Signature		Date	23/8/2022

5 Modelling Particulate Deposition in Gas Turbines Part I: a Non-Spherical Bounce Stick Model

The paper presented below describes the development of a DEM-based model to predict the deposition and rebound of non-spherical particulates in gas turbines. It was validated using a combination of experimental data from open literature and FEA simulations from Chapter 4. It matched or exceeded the modelling capability of existing energy-based bounce stick models as described in Chapter 2.5 while also providing accurate predictions of rebound angular velocity, based on the conclusions presented in Chapter 3. The parametric fitting required to match experimental data was minimal compared to existing approaches, reducing the investment in time and resources required to model deposition involving novel material pairs.

The specification and approach of the model were guided by the results of the previous two chapters: a force-based approach that can predict novel rebound properties like angular velocity for non-spherical particles. The force-based explicit approach was also chosen for its flexibility including additional physical phenomena, if required. This was based on the potential influence of centrifugal forces in the rotating frame of reference, described in Appendix A.

The original, spherical version of the model was presented at the 2021 ASME Turbo Expo. The paper shown below is an adaption that includes the ability to model the collisions of non-spherical particles. It has been submitted to the Journal of Turbomachinery as the first of a two part work that describes the modelling of particulate deposition in CFD. This paper describes an approach to modelling the collision physics, while the second part (Chapter 6) demonstrates its implementation and validation in CFD. The second paper also includes the modelling of surface roughness and how to predict the orientation and angular velocity of non-spherical particles at impact. These are omitted from the first paper as they either require coupling to a fluid solution or are extraneous to the fundamental collision physics.

All work presented in the below paper is that of the thesis author. The FEA simulations used to validate the rebound trajectories of spheroids are taken from Chapter 4, which were also produced by the author. Professors Gillespie and McGilvray supervised the research and are the principal investigators on the project.

DRAFT Modelling Particulate Deposition in Gas Turbines Part I: a Non-Spherical Bounce Stick Model

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The secondary air system and cooling passages of gas turbine components are prone to blockage from sand and dust. Prediction of deposition requires accurate models of particle transport and thermo-mechanical interaction with walls. Bounce stick models predict whether a particle will bounce, stick, or shatter upon impact and calculate rebound trajectories if applicable. This paper proposes an explicit bounce stick model that uses analytical solutions of adhesion, plastic deformation and viscoelasticity to time-resolve collision physics. The Discrete-Element Methods (DEM) model shows good agreement when compared to experimental studies and FEA simulations of micron and millimetre-scale particle collisions, requiring minimal parametric fitting. Non-physical values for mechanical properties, artifices of previous models, are thus eliminated. Further comparison is made to the best resolved and industry standard semi-empirical models available in literature. In addition to coefficients of restitution, other variables crucial to accurately model rebound, for example angular velocity, are predicted. The time-stepping explicit approach allows full coupling between internal processes during contact, and shows that particle deformation and hence viscoelasticity play a significant role in adhesion. Modelling time-dependent internal variables such as wall-normal force allow the modelling of non-spherical particles, the physics of which has been shown by previous work to differ significantly from that of spheres. To date these effects have not been captured well, if at all, by higher-level energy-based models. The spherical version of this bounce stick model has previously been shown to produce good predictions of deposition distribution in CFD. The developments presented here allow the inclusion of more complex collision physics which will improve numerical predictions of deposition in gas turbine components. The accompanying second part to this paper demonstrates this with the addition of surface roughness modelling.

Keywords: Particulate Deposition, Gas Turbines, Bounce Stick Models

NOMENCLATURE

Abbreviations

ARD	Arizona Road Dust
CV	Critical Velocity
DEM	Discrete Element Methods
FEA	Finite Element Analysis
JKR	Johnson, Kendall and Roberts
NH4F	Ammonium Fluorescein
OSU	Ohio State University
TN	Thornton and Ning

Roman Symbols

a	Contact radius, m
a_0	Equilibrium contact radius, m
a_c	Critical pull-off contact radius, m
A_{proj}	Projected area of a prolate spheroid, m ²
a_{ps}	Major semi-axis of a prolate spheroid, m
b_{ps}	Minor semi-axis of a prolate spheroid, m
E	Young's modulus, Pa
F_c	Critical elastic pull-off force, N
F_f	Tangential frictional force, N
F_{n1}	Equivalent elastic normal force, N
F_{nd}	Viscoelastic normal dissipative force, N
G	Shear modulus, Pa
I	Moment of inertia, kg m ²

K	Particle stiffness coefficient from TN model, Nm ⁻¹
k	Stiffness coefficient used in viscoelastic deformation or tangential contact patch deformation, Nm ⁻¹
L_f	Friction moment arm length, m
L_{proj}	Projected length of a prolate spheroid, m
L_{reb}	Rebound moment arm length, m
M_f	Friction moment about particle centroid, N m
M_f	Moment due to friction, N m
M_{reb}	Rebound moment about particle centroid, N m
M_r	Moment due to rolling adhesion, N m
p_y	Limiting surface contact pressure, Pa
R	Particle radius, m
R_{gauss}	Gaussian equivalent radius of curvature at the contact patch, m
V	Velocity, ms ⁻¹
x_0	Characteristic thickness of particle-wall squeeze-film, m

Greek Symbols

α	Prolate spheroid contact patch angle, °
δ_{gap}	Minimum particle-wall separation distance, m
δ_n, δ_t	Normal and tangential contact patch displacement, m
η	Viscoelastic dissipation coefficient, kg s ⁻¹
γ	Surface free energy, J m ⁻²
μ_f	Fluid dynamic viscosity, Pa s
Ω	Angular velocity, rad s ⁻¹
ρ	Particle density, kg m ⁻³
θ	Particle orientation angle with respect to the surface, °
θ_i	Impingement angle, °

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Version 1.19, February 11, 2023

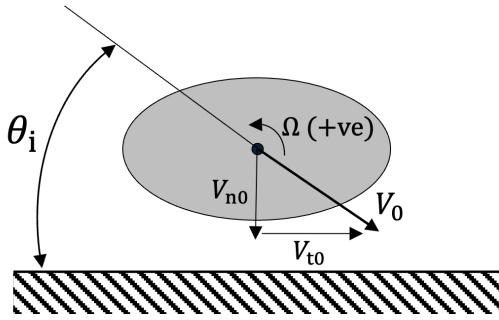


Fig. 1 Particle sign convention.

ξ Adhesive rolling displacement, m

Non-Dimensional Parameters

$\text{CoR}_n, \text{CoR}_t$ Normal and tangential coefficients of restitution

e_0 Equivalent viscoelastic normal coefficient of restitution

$f_{\Delta t}$ Timestep multiplication factor

Stc Collision Stokes number

SF Squeeze-film coefficient δ_{gap}/x_0

Subscripts

0, 3 Far from the wall prior to and following collision

1, 2 Immediately prior to and following collision

e, p, u Elastic, plastic and elastic-adhesive unloading phases of particle deformation

n Normal

r Rebound

t Tangential

Superscripts

* Composite material property or value at the point of maximum deformation

INTRODUCTION

Ingested atmospheric contaminants are known to cause significant damage to gas turbine components through deposition, erosion and corrosion [1]. Upon ingestion, large particles erode compressor aerofoils and hence increase the required design surge margin, limiting whole engine performance. Smaller particles and fragments from these earlier collisions are then transported to the turbine and combustor where secondary air systems and cooling passages are prone to blockage throughout fleet service life. This drives significant increases in maintenance costs and risks failure of hot gas path components. Therefore, the ability to accurately model deposition is desirable to quantify cost of ownership effects and to enable the design of more durable components. Bounce stick models predict whether a particle will bounce, stick or shatter upon collision with a wall and hence are crucial to accurately modelling deposition and transport. The predicted rebound trajectories are equally important to the binary bounce/stick criterion as exposure to different flowfields, particularly in the near wall region, will alter the likelihood and location of subsequent collision and deposition. Comparisons between numerical simulations of particle deposition and experimental observations have shown that while first bounces are well predicted by tracking models, rebound affects the spatial distribution of downstream deposition [2]. Collisions are defined as in Figure 1 with particle rebound trajectories described through normal and tangential coefficients of restitution, CoR_n and CoR_t , defined in Equation 1:

$$\text{CoR}_i = \left| \frac{V_{i3}}{V_{i0}} \right| \quad (1)$$

where $\text{CoR}_n = 0$ implies the particle has stuck. Subscript zero describes the velocity component shortly before collision with the wall. Subscript three describes the velocity shortly after last

contact as described by the explanation of squeeze-film damping in the Methodology section.

Airborne particulates near ground level are predominantly comprised of aluminosilicates [3] and are non-spherical, with aspect ratios between 1.6-1.9 [3, 4]. The size of particulates ingested by the engine is not necessarily representative of those present in the secondary air system as they are often shattered by collisions with compressor blades and larger particles are centrifuged away from compressor bleeds. Therefore, particles at the compressor exit have an average diameter of $6 \mu\text{m}$ [5]. Existing bounce stick models, notably [6–8] assume that particles are cylindrical/spherical to reduce mathematical complexity while taking a high-level approach to modelling, typically defining collision dynamics in terms of kinetic energy losses. While these approaches have been shown to replicate experimental results, the degree of parametric fitting required to do so implies that not all aspects of the collision physics are being accurately modelled. The necessity of fitting to experimental data also limits their use in industry-relevant simulations which consider a range of particle sizes, shapes and compositions. Existing models have also neglected collision-induced rotation (CIR), which was shown by [9, 10] to have a significant effect on micron-scale particle rebound trajectories through the Magnus force. Simulations of deposition in CFD by [10] showed that the exclusion of CIR led to substantial qualitative and quantitative differences in deposition distribution.

Adhesion through van der Waals forces has been shown by [6, 11] to significantly reduce particle CoR_n for diameters less than $10 \mu\text{m}$, particularly where collision normal velocities are low. Other factors that affect particle rebound, also modelled by [6], are plastic deformation and friction with the substrate. Viscoelastic losses have generally not been modelled by previous work, although discussion of the critical velocity model in [7] recognises their importance to predicting CoR_n . It is important to consider not only solid-phase viscoelastic dissipation but also that of the fluid: squeeze-film damping between the particle and surface was shown analytically by [12, 13] to reduce CoR_n towards zero for impacts where both the particle-surface separation gaps and Stokes numbers are small. This is supported by experimental evidence [14] where spheres with $Re < 10$ just before impact failed to rebound, without significant adhesive effects.

A version of this model for spherical particles has already been used by the authors in CFD to predict deposition in gas turbine-representative components [10, 15]. Gaskell et al. [10] validated the qualitative distribution of deposition throughout the domain by comparing to experimental data, demonstrating significant improvements over state of the art energy-based approaches discussed in detail below from Bons et al. [6] and Brach and Dunn [7]. To the authors knowledge, these are the first such experimentally-validated results in the open literature. This demonstrates the utility of the DEM-based approach to the simulation of particle deposition in gas turbine components. Villain et al. [15] applied the spherical DEM model to double wall effusion cooled unit cell geometries. The CFD simulations were able to highlight important and counter-intuitive differences between the susceptibility of two similar designs to particulate damage. The present work builds on the capability of the spherical model, allowing the inclusion of more complex collision physics to CFD. As with the the previous implementation for spheres, examples of potential applications include:

- Prioritising surfaces for corrosion-resistant coatings;
- Identifying regions of the cooling system where deposits may affect the rate of heat transfer;
- Comparing the susceptibility of different geometries to particulate damage.

A methodology for modelling deposition in gas turbines is presented here in two parts. The present work focuses on the development and validation of the bounce stick model itself, while the second part describes its implementation in CFD and validation for predictions of spatially-resolved deposition. The effects of surface roughness are included in the second paper, as surface roughness structures are assumed to be much larger than the diameter of the particle. Therefore, surface roughness will only act to modify the effective angle of incidence and not modify the underlying collision physics, which is the focus of this paper.

Existing Bounce Stick Models. A number of deposition models currently exist in literature that vary in complexity, computational intensity and dependency on empirical data. Most models require at least some parametric fitting, generally to single-particle collision data where the CoR_n and CoR_t of individual particles are measured optically. While this results in accurate predictions of rebound for specific use cases, over-use of fitting means that the model may not be generalisable to novel material pairs, particle sizes, temperatures or shapes. Indeed, applying non-physical corrections to simulation input parameters may negatively impact other aspects of the model. For example modifying the process of plastic deformation may affect predictions of contact area and therefore van der Waals adhesion.

The capabilities of existing models also vary, from those that calculate only a probability of sticking to some that additionally predict rebound trajectories. Here, only those that predict rebound are considered due to the importance of rebound trajectory on the likelihood of subsequent deposition, discussed previously. A variety of existing deposition models are described below.

The Critical Velocity Model. The approach presented in Brach and Dunn [7] uses an assumption of Hertzian contact coupled to the JKR theory of adhesion. It is used most commonly to predict the CoR_n of spherical particle-wall collisions. The model also presents a relation between tangential impulse and rebound angular velocity, however this requires the impulse of the collision to be known *a priori* and hence does not allow predictions of CoR_t and Ω for novel collision cases. The rebound normal velocity V_{n3} is approximated using the work of adhesion W_A and e_0 , the CoR_n in the absence of adhesive and inelastic effects. While the physical significance of e_0 is not discussed by Brach and Dunn, it amounts to a viscoelastic term due to its reliance on collision velocity. The normal rebound velocity can therefore be approximated as:

$$V_{n3} = -e_0 V_{n0} \left(1 - \frac{2W_A}{e_0^2 m V_{n0}} \right)^{\frac{1}{2}} \quad (2)$$

where W_A is positive. The analytical nature of the model, notably the reliance on Hertzian collision physics and the JKR theory of adhesion, leads to highly accurate predictions of CoR_n once e_0 is fitted to experimental collision data. The inability of the model to consider plastic deformation reduces accuracy at high velocities, while the flattened contact pressure distribution during inelastic compression will also invalidate the assumption of Hertzian contact. This would likely only occur where low yield stresses coincide with high surface free energies. Where there remains a tangential slip velocity between the particle and wall throughout contact, a collision in gross-slip, the friction coefficient μ and impulse ratio are identical. This allows an analytical solution for the tangential velocity at rebound:

$$V_{t3} = V_{t0} - \mu (V_{n0} + V_{n3i}) \left(\frac{V_{n3}}{V_{n3i}} \right) \quad (3)$$

where V_{n3i} is the normal rebound velocity while neglecting adhesion. However, Equation 3 is unable to capture the tangential compliance of the contact patch or the transition to particle rolling, so is not accurate for collisions with a velocity vector that is near-normal to the surface.

The OSU Model. The model proposed by Bons et al. [6] took a physics-based approach that included plastic deformation. The particle is treated as a 1D cylindrical spring with a constant stiffness and an empirical correction to allow for spherical geometry. As with the model developed in the present work, the contact time is divided into three stages: elastic compression, plastic compression and adhesive-elastic rebound. Following first contact the particle deforms elastically, storing kinetic energy as elastic potential energy. Following the initiation of plastic deformation, all further deformation is assumed to result in plastic work and no further elastic energy is stored in the particle. During rebound, the stored elastic energy is converted back into kinetic energy. Plastic deformation is assumed to start once a critical normal deformation is reached, $\delta_y = \sigma_y l / E^*$ where l is the length of the cylinder and E^* is the composite elastic modulus. Therefore, the energy available for rebound is expressed by the potential energy stored in the spring at the point of yielding, Equation 4.

$$E_{\text{crit}} = \left(\frac{E^* A}{l} \right) \frac{\delta_y^2}{2} \quad (4)$$

Note that A is the area of each end of the cylinder. If the work of adhesion from JKR theory is greater than this stored potential energy, the particle remains adhered to the surface. If rebound occurs, the energy balance can be used to predict the CoR_n . Bons et al. suggest multiplying W_A by $\sin \theta_i$ to account for the influence of tangential impulse on adhesion. This is shown to improve model accuracy when compared to experimental data, however in the absence of empirical evidence for this correction it is also possible that the sine term is actually correcting for the “semi-empirical” contact area correction.

The tangential coefficient of restitution is modelling using the same basic approach as Brach and Dunn, with an additional $\cos^2(\theta_i)$ term to allow recovery of the CoR_t at high impingement angles (Equation 5). The justification for this is to account for decreased tangential engagement of asperities at normal impingement angles, however the recovery of CoR_t at high θ_i in experimental data where surfaces are smooth implies that it instead mimics tangential compliance of the contact patch:

$$V_{t3} = V_{t0} - \mu (V_{n0} + V_{n3i}) \left(\frac{V_{n3}}{V_{n3i}} \right) \cos^2(\theta_i) \quad (5)$$

The OSU model demonstrates accurate predictions of CoR_n and CoR_t where the input parameters can be tuned to experimental data. Whitaker and Bons [16] present an improved model that accounts for strain rate effects through a variable yield stress and stochastic corrections for particle shape. The parametric approach to modelling non-sphericity may self-incorporate a number of physical phenomena, particularly when it is based on a fundamental method that requires fitting to data. It is therefore limited to the particle sizes, shapes, velocities and possibly flowfields tested (given the potential distributions of particle orientations near the wall). Therefore, the amount of experimental data required to fit an approach for generic collisions of even a single material pair are likely prohibitive.

Virginia Tech Deterministic Models. Critical viscosity methods developed at Virginia Tech are largely empirical, allowing predictions of sticking probability but not necessarily particle rebound [17]. Further work by Tafti and colleagues has developed a series of increasingly complex deterministic models that allow predictions

of particle CoR and rebound angular velocity. First presented by Singh and Tafti [18], an impulse-based approach was shown to produce accurate predictions of CoR_n considering plastic deformation and adhesion. The Jackson-Green model of plastic deformation is used to calculate the rebound velocity in the presence of only plastic deformation. Singh and Tafti then consider adhesive losses separately using JKR theory, based on the approach developed by [7], although experimental validation was limited. The most current model at the time of writing was presented in [8] which includes the effects of surface roughness on plastic deformation and adhesive losses for the first time in the open literature. The model also includes viscoelasticity using an empirically-derived coefficient. Tangential rebound is calculated assuming an empirical coefficient of friction that varies significantly with impact angle, contrasting from an earlier approach by [19] which applied a deterministic, rigid body approach to calculating Ω and CoR_t . The current model was mostly validated using only total CoR so it is difficult to compare with results for other models that report CoR_n and CoR_t separately. The results presented show reasonable agreement to experimental data, however further validation is needed before use in CFD.

Non-Sphericity. Previous work by the authors performed FEA simulations of the collisions between non-spherical particles and a smooth wall [20]. The research aimed to determine the sensitivity of rebound to non-sphericity and identify key differences in the collision physics compared to the spherical case. It is remarkably similar to work presented by Wilson et al. [21] the following year. The rebound of prolate spheroids with an aspect ratio $\text{AR} = 1.9$ were compared with spheres of equivalent volume, validated by experimental data from [22]. Aspect ratio is defined as the area of a circle enclosing the projected area of a spheroid, divided by that projected area. This is shown by the ratio of dark grey to light grey areas in Figure 2 and Equation 6:

$$\text{AR} = \frac{\pi L_{\text{proj}}^2}{4A_{\text{proj}}}. \quad (6)$$

This definition of aspect ratio is chosen to suit the analysis of particle shape from SEM imagery, however it is equivalent to the ratio of major to minor axes $\text{AR} = a_{\text{ps}}/b_{\text{ps}}$. An aspect ratio of 1.9 was chosen based on the mean value from the analysis of atmospheric dust collected at altitude by [3]. Whilst the size and distribution of particles in the secondary air system may not be representative of dust from the wider atmosphere, in the absence of more applicable data, $\text{AR} = 1.9$ was deemed sufficient for the validation of the methodology described herein. The results of the FEA simulations demonstrated that the rebound trajectories of non-spherical particles differed significantly from the similar collisions of spheres and hence should be included in bounce stick modelling. Overall CoR_n was up to 84% lower than an equivalent sphere, while CoR_t was up to 50% greater. The particle angular velocity showed the greatest deviation, changing sign with an absolute value between 5% and 152% of that from an equivalent sphere.

Three fundamental differences in the collision physics were found between spherical and non-spherical particles. The single most important difference was the existence of a rebound moment arm L_{reb} . For a sphere, the line of action of the normal force will always act through the centre of mass of the particle. However, for a spheroid, there may be a tangential displacement L_{reb} between the contact patch and particle centre of mass. This is shown schematically in Figure 3, where the resulting moment $M_{\text{reb}} = F_n L_{\text{reb}}$ acts to oppose the moment due to friction M_f . This causes transfer between linear and angular forms of kinetic energy. The local geometry of the particle at the contact patch will also differ. A particle that collides end-on will have a far smaller effective Gaussian radius of curvature R_{gauss} than one colliding with its long axis parallel to the ground. This is shown in Figure 4, which also defines

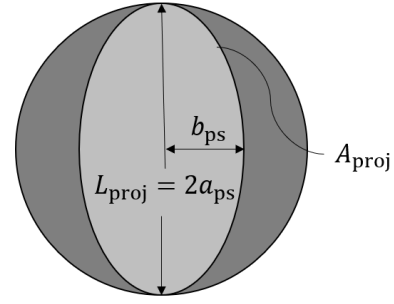


Fig. 2 Projected length and area of a prolate spheroid. Note that A_{proj} is shown in light grey, $L_{\text{proj}}^2 \pi / 4$ is shown in dark grey (see Equation 6).

the particle orientation angle θ and contact patch angle α . The equivalent radius of curvature is defined in Equation 7, originally from [23]:

$$R_{\text{gauss}} = \frac{a_{\text{ps}}^2 b_{\text{ps}}^2}{\left[a_{\text{ps}} \sin(\alpha + \pi/2)^2 + b_{\text{ps}} \cos(\alpha + \pi/2)^2 \right]} \quad (7)$$

whilst α is defined in Equation 8 from inspection of the geometry in Figures 3 and 4:

$$\alpha = \tan^{-1} \left[\frac{-b_{\text{ps}}^2}{a_{\text{ps}}^2} \tan \theta \right]. \quad (8)$$

Finally, multiple collisions may occur between a particle and the wall before it escapes the surface. The angular velocities induced by the rebound moment may be so large that another point on the particle may collide with the surface before it can move sufficiently far away. This is easy to visualise using the collision shown in Figure 4, where a clockwise rotation would cause the right-hand side of the particle to re-collide. During a secondary collision, the angular kinetic energy of the particle is transferred back to a linear form, increasing the overall CoR_n . A fourth, secondary effect of non-sphericity was also found to affect normal contact pressure during the collision. With reference to Figure 3, when the contact patch leads the particle centroid (i.e. $-180^\circ < \theta < -90^\circ$) then the moment due to friction M_f will push the contact patch into the surface. This ‘self-servo’ effect was shown to increase contact pressure, likely influencing plastic deformation and adhesion at small scales. Conversely, where $\theta > -90^\circ$, M_f will act to lift the contact patch away from the surface and reduce pressure.

The simulations discussed above assume a planar impact, where the velocity vectors of the particle lie in the same plane as its major axis. This assumption was made as a body of DNS studies [24–26] have shown that inertial particles are most likely to “tumble” end-over-end rather than “log-roll” near the wall. The model described herein also assumes that the impact is planar for simplicity, which is not expected to present a barrier to accurate simulations of the collision physics in CFD. Incorporating non-sphericity into CFD also presents challenges further to those of the collision itself: predicting the preferential orientation and angular velocity of spheroids at the point of collision. How that is achieved is explained in the accompanying second part of this paper, describing the implementation of this collision model in RANS CFD.

Discrete Element Methods. This paper describes an analytically-explicit bounce stick model based on Discrete Element Methods (DEM). DEM codes are often used to simulate the behaviour of granular assemblies with large numbers of particles, originally

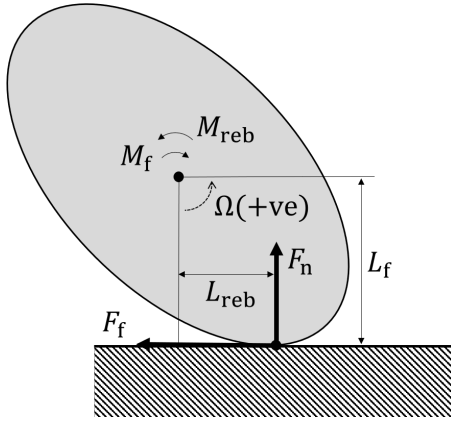


Fig. 3 Schematic of spheroid rebound at $\theta = -135^\circ$.

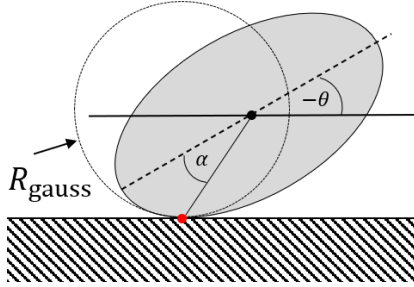


Fig. 4 Particle equivalent radius of curvature R_{gauss} and definition of contact patch angle α .

developed for geotechnical purposes by [27, 28]. The present work will include the effects of adhesion, plastic deformation, friction and viscoelasticity to predict CoR_n , CoR_t and angular velocity, Ω . It differs from most DEM implementations as it only considers single particle collisions between the point of impact with and rebound from a flat, smooth substrate. The model is first derived and experimentally-validated for spherical particles, then extended to model the collision of prolate spheroids with a flat surface. These collisions are validated against the FEA simulations discussed previously.

The DEM-based approach resolves all relevant collision physics throughout the contact time and hence allows coupling between internal variables that is neglected by high-level energy-based models. DEM was also chosen to simulate collisions in the force domain, which suits non-sphericity due to the dependence on the normal force throughout contact, as discussed in the previous subsection. Indeed, it is simple to include any phenomenon that can be expressed in the force domain where full coupling with other internal parameters is guaranteed by the explicit process. This is a key benefit of the DEM approach over energy-based models.

METHODOLOGY

By modelling the forces that act on each particle during the contact time, the equations of motion may be integrated and hence the velocities and displacements during collisions can be found. When modelling deposition in real components, external factors like gas temperature [29, 30] and surface roughness [31, 32] are known to affect deposition rate. Both can be incorporated by modifying the input parameters to the collision model and hence are considered separately in the accompanying second part to this paper. In the case of surface roughness, this involves

a stochastically-augmented angle of incidence [32]. Similarly, assuming the particle and surface materials to be homogeneous and isotropic, mechanical properties can be modified to account for temperature as in [6, 8]. This would include thermochemical effects and phase changes. Post-deposition effects like sintering are out of scope for the present work and should be included in a suitable deposit evolution model. However, deformation of the wall is accounted for through the use of composite elastic moduli like E^* and G^* , and taking the lower of the yield stresses of the particle and substrate material as an input to the simulation. When modelling non-spherical particles, an equivalent radius R is used that is the radius of a sphere with the same volume. The aspect ratio AR is then used to account for non-spherical geometries.

Similarly, erosion and particle fragmentation are not included here hence limiting the scope of the current DEM approach to ductile impacts like those most commonly found downstream of the compressor. As described by Griffith [33], the onset of fracture is governed by the amount of potential energy stored in the particle during compression compared to the fracture energy required to form new crack surfaces. Considering only the region of the particle near the contact patch, as at first contact regions of the particle far from the wall may not experience compressive stress, the stored potential energy is a function of the cube of the contact radius a , i.e. the volume of the area compressed. However, the fracture surface energy is related to the area of the crack surface, proportional to a^2 , leading to a fundamental scaling law that governs crack initiation. Therefore, the ratio of energies that determines the onset of attrition has the dimension of length, usually the diameter of the region of plastic deformation. This means small particles are less likely to shatter than large particles. Hauk et al. [34] performed a theoretical and experimental analysis of the shatter of ice particles. They determined analytically that the collision velocity that initiates cracking $U_0 \propto R^{-2/3}$. Therefore, by fitting experimental data to an empirical coefficient, they were able to predict particle fragmentation for a range of particle diameters and velocities. Taking experimental values of particle attrition velocity U_0 for different materials from Lecoq et al. [35], the velocities at which shatter would be initiated for particles of interest in the secondary air system could be calculated. Lecoq et al. recorded that $400 \mu\text{m}$ diameter NaCl particles suffered fragmentation at a minimum collision velocity of 11 m s^{-1} , while $109 \mu\text{m}$ sand particles fractured at 65 m s^{-1} . Extrapolating the trend from Hauk et al., $10 \mu\text{m}$ particles of NaCl and sand would shatter at 129 m s^{-1} and 319 m s^{-1} . These values are higher than the 100 m s^{-1} flow velocities that are typical of the secondary air system and represent ambient conditions. It is likely that the elevated temperatures would cause the particles to soften and increase the threshold velocity at which attrition initiates. Therefore, it is reasonable to assume that particles present in the secondary air system will not shatter.

When modelling particle motion, it is assumed that the only angular velocity vector is about the axis normal to the page in Figure 1, hence all velocity vectors exist in the plane normal to the wall. The particle equations of motion are shown in Equations 9 and 10:

$$m \frac{d\bar{V}}{dt} = \begin{bmatrix} m \frac{dV_t}{dt} \\ m \frac{dV_n}{dt} \\ 0 \end{bmatrix} = \begin{bmatrix} F_f \\ F_n + F_{nd} \\ 0 \end{bmatrix} \quad (9)$$

$$I \frac{d\Omega}{dt} = M_f + M_r + M_{\text{reb}} \quad (10)$$

where m is the particle mass, F_f is the effective frictional force that acts on the particle, F_n is the normal force that includes elastic and plastic deformation, and adhesive effects, while F_{nd} is the normal

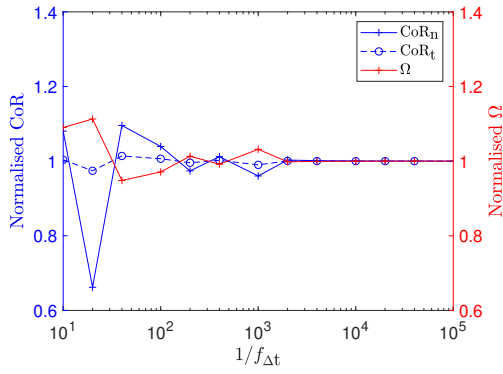


Fig. 5 Sensitivity of CoR_n , CoR_t and Ω to varying timesteps. Results are normalised by the value from the minimum timestep.

dissipative force resulting from viscoelasticity. Note that subscripts n and t alone refer to the values for the particle centroid. The additional subscript c is used to denote the value at the contact patch, which is especially important for non-spherical particles. The normal contact patch velocity is therefore:

$$V_{nc} = V_n + \Omega L_{reb}. \quad (11)$$

In Equation 10, M_f is the moment resulting from effective friction with the surface ($L_f F_f$) and M_r is the moment resulting from adhesion while rolling. Note that, for a sphere, $L_f \equiv R$, as shown by inspection of Figure 3. The simulation timestep Δt is calculated using the particle elastic response time T_c , as in [36]. The elastic response time, an order of magnitude estimation of the total contact time, is multiplied by a factor $f_{\Delta t}$ that is much less than unity to ensure particle deformation throughout the contact time is adequately resolved. This makes the reciprocal of $f_{\Delta t}$ approximately equal to the number of time steps. A series of DEM collision simulations were performed for a generic adhesive, elastic perfectly-plastic microsphere with varying $f_{\Delta t}$ to study timestep sensitivity. These results are shown in Figure 5 where $f_{\Delta t} = 1 \times 10^{-4}$ was deemed the most computationally efficient.

$$\Delta t = f_{\Delta t} T_c = f_{\Delta t} 2R \left(\frac{\rho^2}{V_{n0} E_p^2} \right)^{\frac{1}{5}} \quad (12)$$

Note that E_p is the particle Young's modulus. The tangential force is dependent on the normal force through friction, however the normal force has no such dependency on the tangential. Therefore, the normal force is calculated first during each time step. In most DEM implementations, tangential and normal models are chosen independently of one another and therefore they are presented separately in the following subsections. Where particles bounce multiple times in a single collision event, the collision physics are identical between the bounces (albeit with a greater incoming angular velocity). Therefore, the implementation of a model to predict multiple bounces is discussed separately, in a later section of the paper.

Normal Force Model. The normal force model derived by Thornton and Ning [37], herein referred to as the TN model, is used to calculate the normal force considering adhesion and plastic deformation while the normal dissipative force, accounting for solid-phase viscoelastic effects, is calculated using the model presented in [36]. Squeeze-film effects are modelled using the approach developed in [13], described at the end of this subsection. Adhesion

is based on JKR theory [38] which is widely used for modelling the adhesive behaviour of micron-scale compliant particles. The TN model divides the contact time of an elastic perfectly-plastic adhesive particle into three distinct stages: elastic-adhesive compression; plastic-adhesive compression and elastic-adhesive unloading. These correspond to points 1-2, 2-3 and 3-5 in the normal force vs. normal overlap graph in Figure 6, where arrows show the direction of loading and unloading. Depending on the stage, a different normal stiffness coefficient is calculated and multiplied by the normal displacement at that timestep to obtain the incremental normal force. Throughout the contact time, in every stage, the equivalent elastic normal force at the contact patch is calculated:

$$F_{n,el}(t) = F_{n,el}(t - \Delta t) + \Delta F_{n,el} \\ = F_{n,el}(t - \Delta t) + K_{ne}(t) V_{nc}(t - \Delta t) \Delta t \quad (13)$$

where the elastic normal contact stiffness K_{ne} is a function of the elastic critical pull-off force F_c and the equivalent Hertzian normal force F_{n1} . This is the normal force that would produce the same contact radius a without adhesion:

$$K_{ne}(t) = 2E^* a(t) \left[\frac{3\sqrt{F_{n1}(t)} - 3\sqrt{F_c}}{3\sqrt{F_{n1}(t)} - \sqrt{F_c}} \right] \quad (14)$$

$$F_c = \frac{3}{2} \pi \gamma R_{\text{gauss}} \quad (15)$$

$$F_{n1}(t) = F_{n,el}(t - \Delta t) + 2F_c \pm \sqrt{4F_{n,el}(t - \Delta t) F_c + 4F_c^2} \quad (16)$$

$$a(t) = \left[\frac{3R_{\text{gauss}} F_{n1}(t)}{4E^*} \right]^{\frac{1}{3}} \quad (17)$$

Note that $R_{\text{gauss}} \equiv R$ for a sphere, which is assumed to be constant throughout the collision, γ is the surface free energy and E^* is the composite Young's modulus of the particle and surface materials. The final term in Equation 16 is initially positive, switching to negative once $F_n(t)$ (Equations 13, 22 and 25) is less than or equal to $-F_{cr}$ when unloading (Equations 15 and 23). This is shown by point 4 in Figure 6. At the start of contact, the contact radius is less than the value at yielding, a_y (between points 1 and 2 in Figure 6). Therefore, the particle undergoes elastic-adhesive compression and the actual normal force at contact F_n is equal to the equivalent elastic value $F_{n,el}$:

$$F_n(t) = F_n(t - \Delta t) + \Delta F_{n,el} \quad (18)$$

As calculating a_y directly from Equation 19 is complex, the contact radius at yielding a_y is found using a lookup table. Outside of the time-stepping loop, Equation 19 is solved for a large number of possible values of a_y , linking a range of yield stresses (σ_y) to corresponding yield radii. Using 1D interpolation, a suitable a_y is found using the lower of the yield stresses of the particle and substrate which are inputs to the model. Note that the limiting contact pressure p_y is reached at 2.4 times σ_y [39].

$$p_y = 2.4\sigma_y = \frac{2E^* a_y}{\pi R_{\text{gauss}}} - \left(\frac{2\gamma E^*}{\pi a_y} \right)^{\frac{1}{2}} \quad (19)$$

Where the contact radius a is greater than a_y , yielding occurs (point 2 in Figure 6) and the particle undergoes plastic-adhesive compression between points 2 and 3. Note that the actual normal force F_n and equivalent elastic normal force $F_{n,el}$ diverge here,

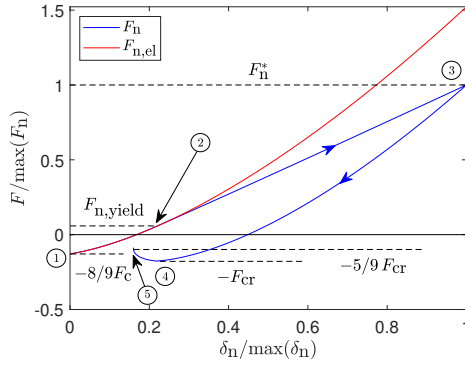


Fig. 6 Normalised normal force vs. normal overlap for the rebound of an adhesive elastic perfectly-plastic microsphere. Arrows show the direction of compression and unloading.

with F_n proceeding on a tangent to the $F_{n,el}$ curve at point 2. To achieve this, a new normal stiffness K_{np} is calculated using the critical contact radius a_c , [37], defined as the contact radius a where $F_n = -F_c$:

$$K_{np}(t) = 3\pi R_{\text{gauss}} p_y - \frac{2a_y E^* [a_c/a(t)]^{3/2}}{3 - [a_c/a(t)]^{3/2}} \quad (20)$$

$$a_c = \left(\frac{9\pi \gamma R_{\text{gauss}}^2}{8E^*} \right)^{1/3} \quad (21)$$

Therefore, the new normal contact force is calculated:

$$\begin{aligned} F_n(t) &= F_n(t - \Delta t) + \Delta F_{np} \\ &= F_n(t - \Delta t) + K_{np}(t) V_{nc}(t - \Delta t) \Delta t \end{aligned} \quad (22)$$

Once the particle normal velocity changes sign at the point of maximum penetration, point 3 in Figure 6, it enters the elastic-adhesive unloading regime between points 3 and 5. If plastic deformation occurs, the contact patch is flattened and hence its effective radius of curvature is increased during unloading. To account for this, a new particle radius R_p is used in place of R_{gauss} in the equations that govern deformation: Equations 15, 16 and 17 to produce F_{cr} , F_{n1r} and subsequent values of a .

$$R_p = \frac{R_{\text{gauss}} F_{n1}^*}{F_n^* + \sqrt{4F_c F_{n1}^*}} \quad (23)$$

Note that F_{n1}^* and F_n^* denote values at the point of maximum penetration, with the latter shown in Figure 6. These values are used to calculate a new contact stiffness K_{nu} and hence the normal force at the contact patch between points 3 and 5:

$$K_{nu}(t) = 2E^* a(t) \left[\frac{3\sqrt{F_{n1r}(t)} - 3\sqrt{F_{cr}}}{3\sqrt{F_{n1r}(t)} - \sqrt{F_{cr}}} \right] \quad (24)$$

$$\begin{aligned} F_n(t) &= F_n(t - \Delta t) + \Delta F_{nu} \\ &= F_n(t - \Delta t) + K_{nu}(t) V_{nc}(t - \Delta t) \Delta t \end{aligned} \quad (25)$$

If yielding does not occur, contact with the surface is broken when $F_n(t) \leq -F_c$ and the particle will rebound along the same force-displacement curve as compression $F_{n,el}$. In effect, the particle stays within the elastic-adhesive compression regime throughout the contact duration and uses only Equations 13, 14 and 18 to calculate F_n . If the contact patch has yielded, as in Figure 6, the sign of $\pm$ in Equation 16 changes when $F_n(t) \leq F_{cr}$ (point 4) and contact is broken when $F_n(t) \geq -5/9 F_{cr}$ (point 5). All force boundary conditions are taken from Table 5.1 in [40]. The increased gradient of the force-displacement curve following the point of maximum penetration F_n^* is due to plastic flattening of the contact patch. Unloading continues until either the particle rebounds, as in this case, or it sticks and dissipates its kinetic energy through viscoelastic dissipation while oscillating.

The normal dissipative force that accounts for solid-phase viscoelastic effects F_{nd} is calculated by multiplying a dissipation coefficient η_n by the particle normal velocity V_n :

$$\eta_n(t) = \alpha \sqrt{m k_n(t)} \quad (26)$$

$$k_n(t) = \frac{4}{3} E^* a(t) \quad (27)$$

where α is a sixth-order polynomial fit to an analytical solution of e_0 , the CoR_n if viscoelasticity were the only dissipation mechanism in a normal contact [36]. The value of e_0 is an input to the model, currently fit to experimental observations. This is the only explicit parametric fitting included in the model. However, its implementation allows physically-representative normal forces throughout the contact time, based on the analytical nature of the approach taken by Marshall [36]. Note that the lowercase k_n is distinct from the stiffness coefficients used in the TN model. Once F_n and F_{nd} are known for each time step, the normal components of the particle equations of motion in Equation 9 can be updated and the normal force can be used as an input to the tangential contact model.

Squeeze-film damping is the result of fluid motion between the particle and wall during approach and rebound, reducing the particle velocity magnitude shortly before and after the collision. As the effect primarily occurs shortly before first contact and after rebound, which define the beginning and end of the DEM time-stepping loop, it is used to modify the input and output velocity vectors of the DEM as described below. Therefore, particle velocities at first and last contact with the surface are defined as V_{n1} and V_{n2} while values far from the wall before and after the collision are defined as V_{n0} and V_{n3} . Therefore, V_{n0} and V_{n3} are the input and output velocity vectors to the simulation while V_{n1} and V_{n2} are effectively internal variables. The magnitude of the squeeze-film effect depends on the collision Stokes number Stc :

$$Stc = \frac{2\rho V_{n0} R}{9\mu_f} \quad (28)$$

where μ_f is the fluid dynamic viscosity. A smaller value of Stc implies greater influence of fluid viscosity on particle motion and hence a greater reduction in velocity. Expressions that relate V_{n0} to V_{n1} and V_{n2} to V_{n3} were derived by [13]:

$$\frac{V_{n1}}{V_{n0}} = 1 + \frac{1}{Stc} \ln(\delta_{\text{gap}}/x_0) \quad (29)$$

$$\frac{V_{n2} - V_{n3}}{V_{n0}} = \frac{1}{Stc} \ln(\delta_{\text{gap}}/x_0) \quad (30)$$

where δ_{gap} is the minimum separation distance, which for practical purposes is surface roughness, and x_0 is the squeeze-film thickness which is generally equal to $0.01R$ [41].

Table 1 NH4F particle and substrate materials properties from [11] and [42].

	NH4F	Molybdenum	Silicon
E (GPa)	1.2	330	182
Poisson's Ratio	0.33	0.38	0.28
Density (kg m^{-3})	1350	-	-
γ (J m^{-2})	-	0.34	0.38
σ_y (MPa)	74	-	-

Tangential Model. The tangential forces that act at the contact patch are calculated using the widely-used model proposed by Cundall and Strack [28] with additional equations from [43] to account for rolling adhesion. The tangential collision model was chosen based on the comparisons made by [44], which conclude that a constrained linear spring model provides the most accurate predictions of tangential rebound. The slip velocity between the particle and surface V_s is key to the direction of frictional force. Here, the slip velocity will initially be positive where the frictional force is initially negative:

$$V_s(t) = V_t(t) + L_f \Omega(t) \quad (31)$$

noting that angular velocity Ω is negative in the clockwise direction, hence ensuring $V_s < V_t$. Cundall and Strack's model incorporates a spring and dashpot to model tangential deformation at the contact patch with a slider to account for frictional effects. Therefore, the tangential force at the contact patch F_f is calculated using Equations 32 and 33:

$$F_f(t) = \min [|k_t(t) \delta_t(t) + \eta_t V_s(t)|, -\mu |F_n(t) + 2F_c|] \quad (32)$$

$$\delta_t(t) = \delta_t(t - \Delta t) - V_s(t) \Delta t \quad (33)$$

where $k_t(t) = 8G^* a(t)$ is the tangential stiffness, μ is the coefficient of friction and $\eta_t = \eta_n$. The rolling adhesion model from Dominik and Tielens [43] uses a rolling displacement ξ as defined below to calculate the moment due to adhesion that opposes the particle's angular velocity. This moment is due to an asymmetrical pressure distribution between the front and rear of a rolling particle as points at the rear "jump-off" the surface at a higher normal overlap than those at the front "jump-on". Therefore, when rolling the contact patch lags behind the centroid and the rolling displacement is the tangential projection of the distance between the centre of the contact patch and the particle centroid. Below a critical value ξ_{crit} , the contact patch remains stuck. Once $\xi = \xi_{\text{crit}}$, the contact patch begins to move at the same tangential velocity as the centroid, lagging ξ_{crit} behind. Clearly, there is coupling between ξ and the tangential contact patch deformation δ_t in Equation 32. However, to reduce complexity it is assumed that the two models work independently with ξ defined as the time integral of the rolling velocity $V_L = R \Omega$, limited in magnitude to ξ_{crit} . Therefore, the moment due to adhesive rolling M_r is given by:

$$M_r(t) = -4F_c \xi(t) \left(\frac{a(t)}{a_0} \right)^{\frac{3}{2}} \quad (34)$$

$$a_0 = \left(\frac{9\pi \gamma R_{\text{gauss}}^2}{E^*} \right)^{\frac{1}{3}} \quad (35)$$

where a_0 is the equilibrium contact radius. The critical rolling displacement is often expressed as the critical rolling angle $\theta_{\text{crit}} = \xi_{\text{crit}}/L_f$, shown experimentally by [45] to be between $19 - 64 \times 10^{-3}$ rad for micron-scale polymer spheres. The rolling resistance model by Dominik and Tielens was also shown to produce good approximations of the tangential force.

RESULTS

To validate different aspects of the normal and tangential collision models, the predictions of the DEM code are compared with separate sets of experimental and numerical data. To validate the normal adhesive and plastic deformation predictions of the TN model, the DEM is compared with the rebound of adhesive microspheres undergoing entirely normal collisions in the following subsection. This is to provide a simple first case to ensure that the most important aspects of the collision physics are modelled correctly. For the same reason, the tangential model and plastic deformation predictions of the TN model are validated using collision data from the oblique impacts of millimetre-scale spheres [22]. Validating angular velocity predictions with large particle is essential, given the limitations of optical measurement techniques for micron-scale particulates. Rolling adhesion is considered separately given the reduced dependency of rebound on adhesive effects for diameters $\gg 10 \mu\text{m}$ [46].

For the validation of non-spherical collisions, DEM predictions are compared with the FEA simulations of millimetre-scale particles discussed in the Introduction. This is due to the lack of particle-by-particle data for important rebound characteristics like angular velocity. Comparison with FEA also allows fluid effects to be excluded, as experimental datasets like those from [30, 47] involve the particle being fired at high velocity at an impingement plate. As discussed previously, spheroids may exhibit preferential orientations in turbulent flow which are not captured in the experimental data. Hence, such datasets would require coupling to a CFD solution, as described in the accompanying second part to this paper.

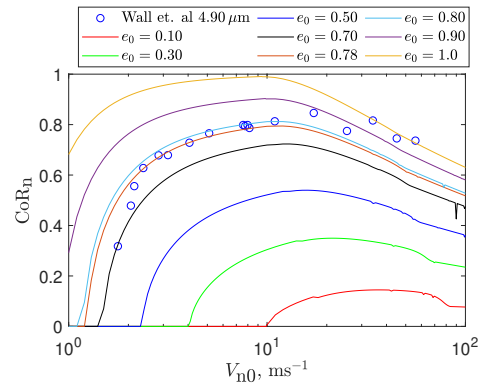


Fig. 7 Normal collisions of 4.90 μm NH4F spheres and a Molybdenum substrate for varying viscoelasticity, experimental data from [11].

Normal Collisions of Microspheres. The results of the DEM bounce stick model are compared with the experimental data from Wall et al. [11] to validate the modelling of adhesive effects. The TN model was compared with this data by Ning [40] and Xie et al. [42], which required a dynamic yield stress to match experimental data (a similar technique to Bons et al. [6] and Whitaker and Bons [16]). Ning showed that the yield stress varied from approximately 40 MPa at a normal impact velocity of 1 ms^{-1} to approximately 145 MPa at 30 ms^{-1} and above. In [16], Whitaker and Bons

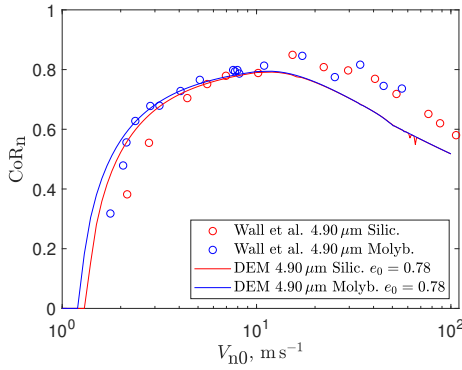


Fig. 8 Normal collisions of 4.90 μm NH4F spheres [11] with Molybdenum and Silicon substrates.

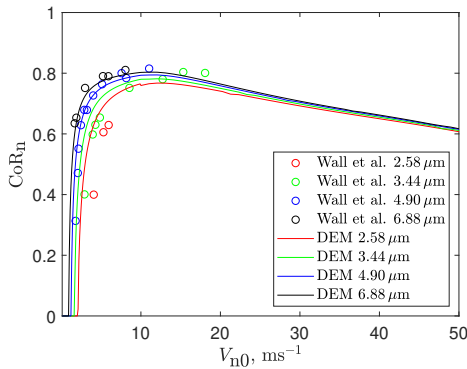


Fig. 9 Normal collisions of NH4F microspheres with a Molybdenum substrate, $e_0 = 0.78$, $SF = 0.1$. Experimental data from [11].

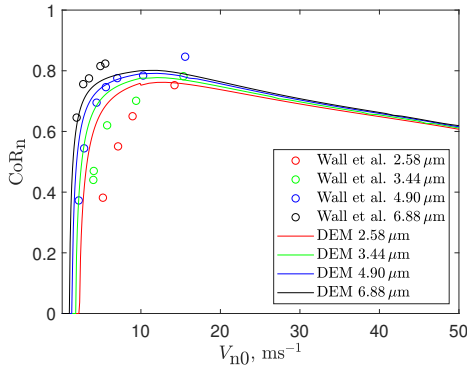


Fig. 10 Normal collisions of NH4F microspheres with a silicon substrate, $e_0 = 0.78$, $SF = 0.1$. Experimental data from [11].

present a compelling argument for strain rate effects affecting the yield stress used in modelling. As they explain, for some materials the onset of plastic deformation is known to be dependent on the rate at which the material is deformed [48]. However, the variation modelled by Ning seems extreme. Neither the TN model nor Whitaker and Bons explicitly include viscoelasticity, but rather match physical phenomena related to strain rate by varying the yield stress. In this paper the impact of different viscoelastic dissipation coefficients η_n is studied to provide a more robust explanation of the experimental dependence on strain rate.

The effects of squeeze-film damping are also considered with two values of minimum separation gap δ_{gap} considered, which is analogous in this context to surface roughness height.

In [11], ammonium fluorescein spheres, herein referred to as NH4F, between 2.58 μm and 6.88 μm in diameter were accelerated towards a flat plate at a normal angle of incidence. Total velocity varied between 1 – 100 ms^{-1} . Different substrate materials were used, with silicon and molybdenum considered here. Material properties for the particles and substrates are shown in Table 1. Note that γ is only shown for substrates as it depends on the particle-substrate material pairs, density is only shown for the particle as substrate mass is not relevant and it is assumed that, for these material pairs, the particle will always deform before the substrate hence only the particle yield stress is shown. The minimum separation gap δ_{gap} was set to 1×10^{-9} m for the results shown in Figures 7 – 10, a similar value to that used in [13] for the same experimental data. Additional simulations were also run for $\delta_{\text{gap}} = 1 \times 10^{-10}$ m which, although unfeasibly smooth in reality, demonstrates the upper limit of the squeeze-film effect through the dependence on the ratio δ_{gap}/x_0 in Equations 29 and 30. The two squeeze-film conditions are therefore referred to as $SF = 0.1$ and $SF = 0.01$ respectively where SF is the ratio δ_{gap}/x_0 . The dynamic viscosity of the air surrounding the particle was set to 1.5×10^{-5} Pa s as in [13].

As described in the Methodology section, the normal viscoelastic dissipation coefficient η_n is calculated using e_0 , equivalent to the CoR_n if viscoelasticity were the only dissipation mechanism in a normal collision. DEM predictions of CoR_n were generated for 4.90 μm NH4F spheres impacting a molybdenum substrate with different values of e_0 , shown in Figure 7. Simulations ran for approximately 25,000 iterations. CoR_n is shown to have a significant dependence on viscoelasticity, through e_0 , with CoR_n varying between near unity and zero between $e_0 = 1.0$ and 0.10. Notably, the TN model is able to match experimental data well with a constant yield stress when $e_0 = 0.78$. In addition to direct viscoelastic dissipation, an additional viscoelastic phenomenon leads to adhesive energy dissipation. During an elastic collision, the particle behaves as a spring storing elastic potential energy. Therefore, at the point where first contact is made, the point of zero normal overlap, the particle should have approximately the same magnitude of normal velocity on rebound and incidence, assuming small losses due to direct viscoelastic dissipation. However, with adhesive contact the particle remains adhered to the surface past zero normal overlap during rebound, “necking” as kinetic energy is transferred back to elastic potential energy. It is this elastic spring that provides the necessary potential energy to overcome the adhesive potential and allow rebound. Hence, the adhesive process is heavily dependent on particle deformation at a point of high normal velocities, noting that the normal dissipative force F_{nd} is the product of η_n and V_n .

DEM predictions of CoR_n for a silicon substrate are also shown in Figure 8, where $e_0 = 0.78$ was found to produce the best fit to experimental data. This fit was obtained using only the mechanical properties provided by [11, 42], without further fitting of σ_y to the results. The DEM correctly predicts a higher sticking velocity of the NH4F-silicon pair, given the higher surface free energy between the two. The coefficients of restitution converge when in the plastic deformation regime, as is also the case for the experimental data. Further simulations are shown in Figures 9 and 10, where the particle diameter ranges from 2.58 – 6.88 μm for molybdenum and silicon substrates respectively. The critical sticking velocity increases with particle diameter, matching the results of existing bounce stick models [6, 7]. The value of e_0 was calibrated for 4.90 μm particles, so while CoR_n matches these data extremely well the DEM tends to over-predict CoR_n for smaller particles and under-predict CoR_n for larger diameters. At

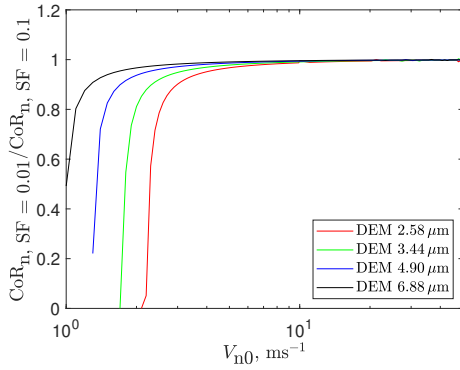


Fig. 11 Effect of different levels of squeeze-film damping on normal Coefficient of Restitution (CoR_n) for the collisions shown in Figure 9.

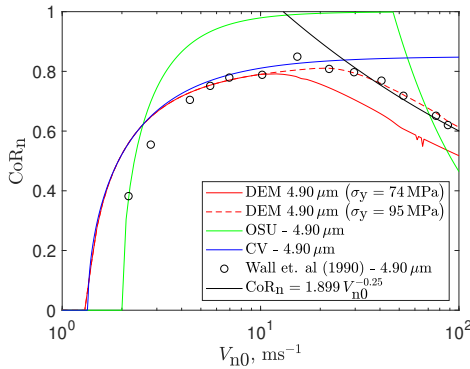


Fig. 12 Comparison between the DEM, OSU [6] and Critical Velocity (CV) [7] deposition models for 4.90 μm NH4F particles vs. silicon.

SF = 0.1 squeeze-film damping clearly arrests the motion of small particles disproportionately, due to the dependence on collision Stokes number, Equation 28, providing a possible explanation for the discrepancy between modelling and experimental data. To understand the sensitivity to SF, it was reduced by an order of magnitude to 0.01: the ratio of the coefficients of restitution for different values of SF is shown in Figure 11. Whilst the normal coefficients of restitution predicted are largely unchanged with greater damping (ratio ≈ 1), the magnitude of the effect is greater as particle diameter decreases and as the normal velocity approaches the stick velocity $\text{CoR}_n = 0$ for all particles. Indeed, excluding the squeeze-film effects entirely from Figure 9 does not significantly improve the fit to data, especially if the value of e_0 is adjusted to compensate. It is also noteworthy that these particles are relatively smooth and spherical, meaning the effects of squeeze-film damping are likely stronger here than for the rough, non-spherical particles encountered in engines.

The DEM predictions of CoR_n match the key features of experimental results for a range of particle diameters and collision velocities considering adhesive, viscoelastic and inelastic effects. Squeeze-film damping is seen to have only a small effect on the normal coefficient of restitution. It is therefore recognised that the model fails to capture another diameter-related phenomenon which affects particle motion. While it might be possible to use both a velocity dependent yield stress and variable viscoelastic coefficient to perfectly replicate particle rebound, suitable physical bases for doing so are not yet apparent. As a key motivation for

the development of the model is to allow its application to different particles without empirical tuning this has not been undertaken.

Comparison to Existing Models. Predictions of CoR_n from DEM were compared with those from The Ohio State University (OSU) model [6] and the Critical Velocity (CV) model [7]. As explained previously, these models are primarily energy based and require some degree of empirical tuning using bespoke material properties. When comparing the predictions of largely empirical models and those of the predominantly deterministic DEM method, it is important to consider how these approaches may be used in industrial simulations of particle deposition: extensive collision rebound data are unlikely to be available, especially for novel material pairs. Hence, models should prioritise the use of published materials data and minimise empirical corrections. Predictions from the energy-based methods presented here are, therefore, generated using optimised input parameters that are constant over the full range of collision velocities modelled. This allows the fidelity of the models' physics to be assessed independently of the quality of available material properties. The same procedure has been used to optimise e_0 in the DEM model and thus provides a fair comparison between methods.

Two primary parameters that influence CoR_n are γ and σ_y , which define both loss mechanisms that affect normal rebound velocity in the OSU model: plastic deformation and adhesion. These were optimised against 4.90 μm NH4F spheres vs. a silicon substrate from [11] as this presented the largest range of collision velocities available. Yield stress is also explicitly tuned in [6, 46] while γ is not well reported in literature. The optimised values were defined as those which generated a minimum average error between model predictions and experimental data in the range $0.1 \text{ MPa} \leq \sigma_y \leq 100 \text{ MPa}$ and $0.01 \text{ Jm}^{-2} \leq \gamma \leq 1 \text{ Jm}^{-2}$. One thousand samples were taken of both γ and σ_y to produce a 10^6 element map of CoR_n . A global least squares minimisation yielded $\sigma_y = 67.2 \text{ MPa}$ and $\gamma = 0.0536 \text{ Jm}^{-2}$. The same procedure was followed for the CV model, where the parameters optimised were $\gamma = 0.328 \text{ Jm}^{-2}$ and $e_0 = 0.848$. The notable discrepancy in γ between the OSU model and other approaches arises from a difference in calculations of assumed maximum contact area, the OSU model taking an empirical approach that predicts larger values than Hertzian methods when using the constants a , b , and c supplied by [6].

The predictions of CoR_n for 4.90 μm spheres using each model with the optimised parameters are shown in Figure 12. Here the value of σ_y used in the DEM model was optimised to 95 MPa. The performance of the CV and DEM models at low velocities are very similar, owing to their shared use of Hertzian contact models. The CV model's use of an empirical CoR_n in the absence of adhesion, e_0 , approximates viscoelastic behaviour, though it is not physically modelled as in the DEM, instead being employed as an empirical correction. As plastic deformation is neglected, the CV model fails to accurately predict the drop in CoR_n at high velocities. By contrast, the OSU model predicts plastic deformation but the inability to account for strain-rate effects when a constant value of σ_y is used reduces accuracy at intermediate collision velocities. Analytical solutions of collision energetics, [38, 49] show that CoR_n is proportional to $V_{n0}^{-0.25}$ during highly plastic deformation, confirmed by several experimental studies summarised in [40]. This trend is plotted in Figure 12, fitted to the experimental data point at the highest velocity $V_{n0} \approx 90 \text{ ms}^{-1}$. The plastic behaviour is close to DEM predictions, however the gradient of the OSU CoR_n is significantly steeper than the analytical relationship. Using a constant σ_y and γ , there does not appear to be a close fit of the OSU model to experimental data. However, this was accounted for using a velocity dependent σ_y fit in [46]. Overall, the performance

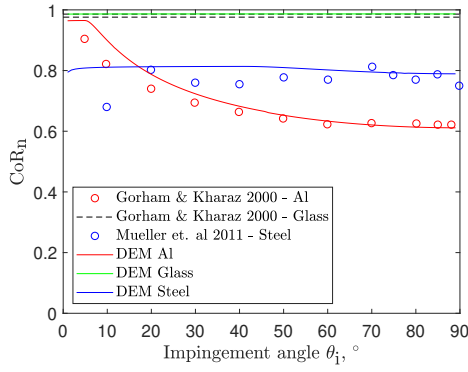


Fig. 13 Normal coefficients of restitution of millimetre-scale particles, experimental data from [22, 50]. Dashed lines show experimental range.

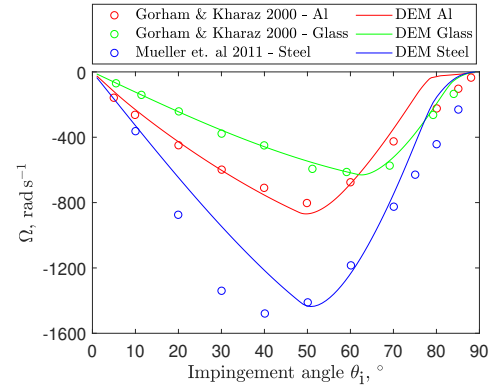


Fig. 15 Rebound angular velocity of millimetre-scale particles, experimental data from [22, 50].

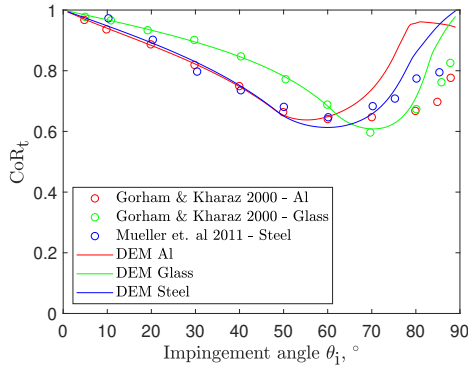


Fig. 14 Tangential coefficients of restitution of millimetre-scale particles, experimental data from [22, 50].

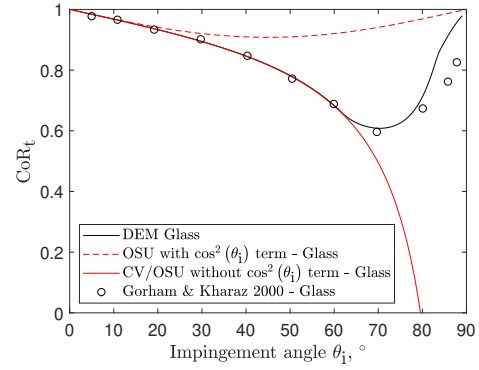


Fig. 16 Predicted CoRt for DEM vs. OSU [6] and Critical Velocity [7]. Experimental data from [22].

of DEM is shown to be favourable compared to existing models where optimised values are held constant over a range of collision velocities.

Millimetre-Scale Sphere Collisions. The collisions of millimetre-scale particles were simulated to validate the tangential model [28] using experimental data from [22, 50]. Large alumina particles 5.0 mm ($V_0 = 3.9 \text{ ms}^{-1}$) and 1.8 mm ($V_0 = 2.3 \text{ ms}^{-1}$) in diameter ensure sphericity and allow comparison between experimental and numerical angular velocities at rebound, as experimental techniques prohibit measurements for micron-scale particles. As the particles are large, squeeze-film effects are likely to be negligible and hence neglected. Particle and substrate materials properties are shown in Table 2. All simulations were run with $\gamma = 0.3 \text{ Jm}^{-2}$ as the value is likely to be of order unity, although the effects of adhesion are small at this scale.

The rebound properties of the millimetre scale particles are shown in Figures 13-15. The DEM predictions of normal coefficient of restitution in Figure 13 show good agreement with experimental data. Increasing plastic deformation with more normal collisions is modelled well in the aluminium substrate case, while the DEM correctly predicts elastic collisions with a glass substrate, the CoR_n being close to unity. Rebound in the alumina-steel case is largely driven by viscoelasticity where $e_0 = 0.75$, with negligible plastic deformation demonstrated by the lack of dependency on normal velocity at high impingement angles. This is consistent with the description of the alumina-steel collisions in [50] as “elastic-dominant”. Values of e_0 for the aluminium and glass cases were 0.95 and 0.98 respectively,

within the range of $0.90 < \text{CoR}_n < 1.0$ shown by [54] to be responsible for reductions in CoR_n related to viscoelastic losses and elastic wave propagation. While e_0 for the alumina-steel collisions is much lower than that of the alumina-aluminium and alumina-glass impacts, the near constant CoR_n with impingement angle and apparent lack of plastic deformation makes it likely that only viscoelasticity is responsible, given the size of the particles precludes adhesive effects. It is possible that material fracture is responsible, which is not considered in the present model. The value of σ_y for glass in Table 2 was taken as 10% of the maximum theoretical value presented in [51], as the author acknowledges that small surface areas will have higher strengths than typical values used in design.

Predictions of CoR_t in Figure 14 show excellent agreement at oblique impact angles, where the particle slides throughout the duration of the impact, however the DEM diverges from experimental data at impact angles close to normal. Excellent agreement is shown in the elastic glass and steel substrate cases, while comparison with CoR_n in Figure 13 indicates that increasing plastic deformation reduces the ability of Cundall and Strack’s model to accurately model CoR_t . As described by [44], when using normal force models that consider plastic deformation the tangential spring in Equation 32 may not always be constrained by Coulomb friction (μF_n). Therefore, adaption of Cundall and Strack’s model will be considered in further work to improve CoR_t accuracy at near-normal angles of incidence. Angular velocity is well predicted by the DEM, as shown by Figure 15. Agreement is best where substrate and particle material properties are provided with experimental rebound data, as is the case for the aluminium and glass collision. As described by [9, 55], the

Table 2 Particle-substrate material properties.

	Alu- mina	Float Glass	Al7178	Hard. Steel
E (GPa)	360	70.0	73.1	-
G (GPa)	-	-	-	80.0
Poisson's Ratio	0.23	0.25	0.33	0.29
Density (kg m^{-3})	3500*	-	-	-
σ_y (MPa)	-	1700	470	1320
μ	-	0.0920	0.180	0.163
References	[22]	[22, 51]	[22, 52]	[50, 53]

* porosity = 0.68 for hardened steel cases

location of peak angular velocity in Figure 15 is largely governed by elastic materials properties. Where these are not provided with experimental data and hence must be found elsewhere, e.g. the steel substrate case, less accurate predictions can be made.

Overall, the DEM is shown to accurately predict CoR_n , CoR_t and Ω for different materials pairs considering viscoelasticity, friction and plastic deformation. Data matching, conducted to estimate η_n at a single particle size appears to scale robustly throughout the data. The model is highly sensitive to material properties and future extensions should address the applicability of Cundall and Strack's tangential model to better predict CoR_t at the most normal impingement angles where plastic deformation is significant.

Comparison to Existing Models. The OSU model adopts the impulse-based tangential modelling strategy from the CV approach [7]. At oblique impingement angles where the particle slides throughout the contact duration, this is an analytical solution. DEM predictions of tangential restitution were compared to those of the OSU model, with and without the empirical $\cos^2(\theta_i)$ correction proposed by the authors. Angular velocity was not compared as this was not modelled by [6, 46]. Model predictions were generated for the alumina-glass collision case shown above, from [22]. Material properties were not optimised as in the previous subsection because the experimental data has no significant dependence on σ_y or γ . Results are shown in Figure 16, where both modelling approaches accurately predict CoR_t at low impingement angles where the particle slides throughout the duration of contact. However, the simple impulsive approach applied by the OSU and CV models is unable to capture the transition from sliding to rolling or the tangential compliance of the contact patch at higher impingement angles [44]. The empirical $\cos^2(\theta_i)$ term reduces overall model accuracy and does not appear to represent the underlying collision physics. The DEM model performs favourably when compared to existing models, especially at high impingement angles.

Rolling Adhesion. Rolling adhesion reduces the magnitude of the particle tangential velocity by reducing the angular velocity, as shown in Equations 10 and 34. Due to the difficulties in measuring the angular velocity of micron-scale particles, it is not possible to directly compare DEM predictions of rolling adhesion with experimental data. However, as previously discussed, [45] found that the rolling adhesion model of Dominik and Tielens [43] showed good agreement with experimental measurements where micron-scale particles were rolled along a surface with a stylus.

Here, the effect of rolling adhesion is shown for a $10\text{ }\mu\text{m}$ diameter particle of ARD using materials properties from [6] at $\theta_i = 45^\circ$ and $\gamma = 0.8$. The critical value of rolling displacement $\xi = \xi_{\text{crit}}$ is set to $0.06R$ to match the experimental observations of micron-scale particles by [45]. A comparison between the rolling and tangential velocities of the particle while sticking is shown in Figure 17. The particle initially slides along the surface until the

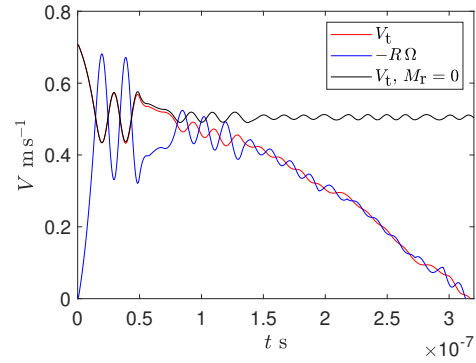


Fig. 17 Tangential and rolling velocities of a $10\text{ }\mu\text{m}$ ARD particle during a sticking collision.

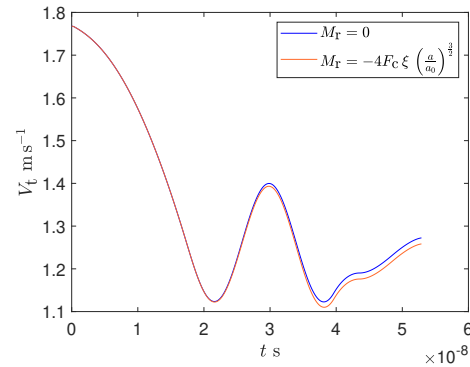


Fig. 18 Tangential velocities of a $10\text{ }\mu\text{m}$ ARD particle during bouncing collisions with and without rolling adhesion enabled at $\theta_i = 45^\circ$.

tangential and rolling velocities are matched, at which point the contact patch enters microslip at approximately $t = 0.3 \times 10^{-7}\text{ s}$. In this regime, the contact patch oscillates akin to a spring-dashpot system as described by Cundall and Strack with the oscillations damped by friction and tangential viscoelasticity, leading the particle to roll according to rigid body motion. As the slip velocity between the particle and wall reduces, the rolling adhesion moment M_r , Equation 34, becomes the dominant source of tangential friction and hence is responsible for the particle coming to rest. This is demonstrated by the near constant tangential velocity of the particle when rolling once rolling friction is disabled, also in Figure 17. However, the distance a stuck particle rolls after impact is not relevant to broader bounce stick modelling, only the effect of rolling adhesion on CoR_t is important. The effects of rolling adhesion on tangential velocity will increase with collision time, given ξ is the time integral of the rolling velocity. As, through impulse, the largest collision time will be at the lowest possible normal velocity at which rebound still occurs, simulations were performed at $\theta_i = 45^\circ$ just above the critical velocity of 2.4 m s^{-1} with and without rolling adhesion enabled. The results are shown in Figure 18 where the collision time is much less than that taken for the particle to come to rest in Figure 17. Rolling adhesion has only a small effect on tangential velocity at rebound and hence CoR_t is 1.2% lower than with rolling adhesion at 0.711 vs. 0.719. It should also be noted that ξ reached a maximum value of only $0.14\xi_{\text{crit}}$, reducing the sensitivity of the DEM approach to experimental observations from [45]. Therefore, while it is not possible to quantitatively validate the modelling of rolling adhesion, the implementation here shows the correct qualitative behaviour using a

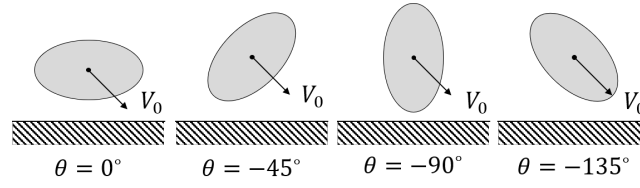
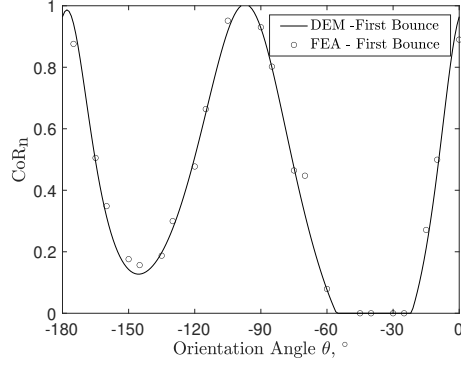
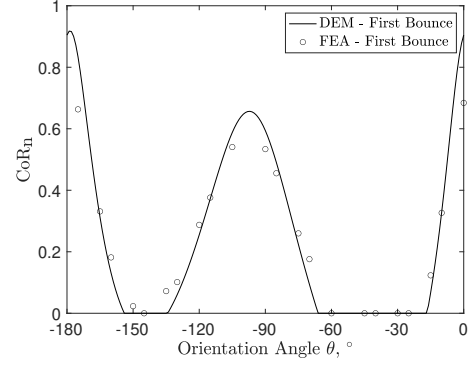


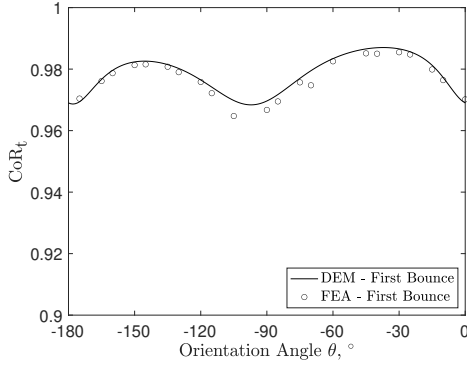
Fig. 19 Key of particle orientation angles.



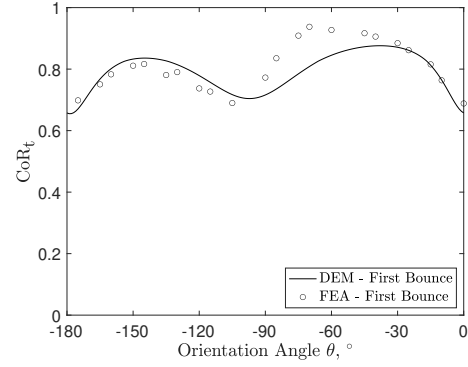
(a) Normal coefficient of restitution CoR_n . Note that, here, $CoR_n = 0$ means that the particle is still moving towards the wall following the first collision.



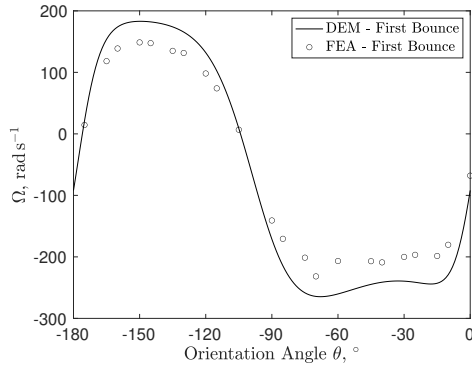
(a) Normal coefficient of restitution CoR_n . Note that, here, $CoR_n = 0$ means that the particle is still moving towards the wall following the first collision.



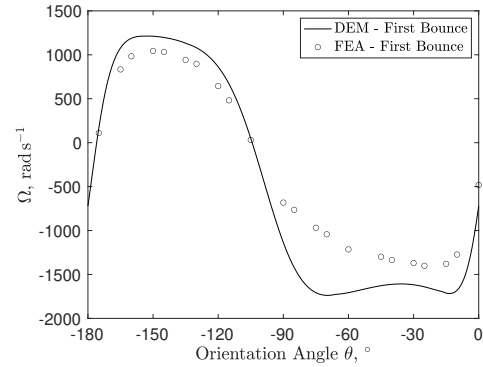
(b) Tangential coefficient of restitution CoR_t .



(b) Tangential coefficient of restitution CoR_t .



(c) Rebound angular velocity Ω .



(c) Rebound angular velocity Ω .

Fig. 20 DEM predictions of non-spherical primary particle rebound vs. FEA from [20]. Particles are 5 mm diameter equivalent alumina ellipsoids impacting an aluminium substrate with $\theta_i = 5^\circ$.

Fig. 21 DEM predictions of non-spherical primary particle rebound vs. FEA from [20]. Particles are 5 mm diameter equivalent alumina ellipsoids impacting an aluminium substrate with $\theta_i = 45^\circ$.

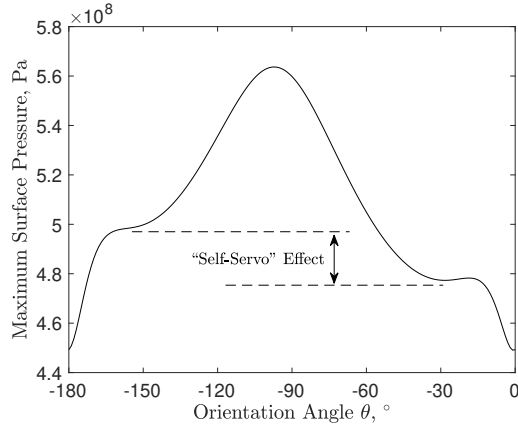
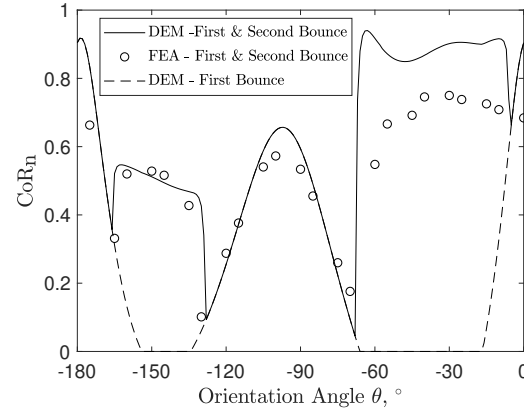


Fig. 22 Contact patch maximum contact pressure vs. particle orientation. Ellipsoid $\theta_i = 45^\circ$.

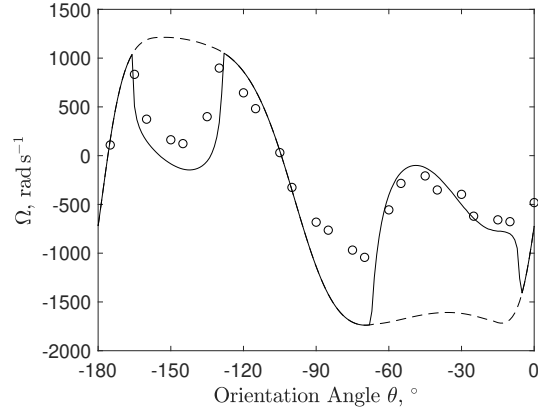
model that has been shown to match experimental data for adhesive rolling moments. In addition, in the limiting case applicable to gas turbine particulates the effect on CoR_t was found to be small.

Non-Spherical Rebound. The ability of the DEM model to predict the rebound of non-spherical particles is assessed with reference to the FEA simulations discussed previously, from [20]. They model the rebound of alumina prolate spheroids with $\text{AR} = 1.9$ and an equivalent spherical diameter of 5 mm. The particles collide with the aluminium substrate at one of two impingement angles, $\theta_i = 5^\circ$ and $\theta_i = 45^\circ$ to assess the performance of the model in a predominantly elastic and elastic perfectly-plastic regime respectively. While the ability of the model to predict adhesion is not explicitly validated here, due to the size of the particles, the previous validation serves to ensure that adhesive forces would be applied correctly to micron-scale spheroids. The performance of the FEA simulations was validated [20] by simulating the rebound of 5 mm spheres from Gorham and Kharaz [22], the same dataset used previously to validate DEM predictions of CoR_n , CoR_t and Ω . For each impingement angle, approximately 22 FEA simulations of primary particle impact were performed at different orientations to the surface θ . A key showing impacts with different θ is shown in Figure 19, which is formally defined in [20]. Primary impacts are here described as the first collision of the particle with the surface, neglecting any subsequent secondary collisions once the contact patch has initially rebounded from the surface.

The primary rebound properties predicted by the DEM model are compared with the FEA results in Figures 20 and 21 for impacts at an impingement angle $\theta_i = 5^\circ$ and $\theta_i = 45^\circ$ respectively. The $\theta_i = 5^\circ$ case in Figure 20 is elastic, as demonstrated by the normal coefficient of restitution that approaches unity. The DEM model is shown to produce highly accurate predictions of primary bounces for CoR_n , CoR_t and Ω , implying that all relevant collision physics have been incorporated and successfully coupled to one another. This is supported by Figure 22, which shows the maximum contact pressure at different particle orientations. The higher surface pressure on the left of the graph, where $\theta < -120^\circ$, compared to the right is due to the “self-servo effect” described in the Introduction. This demonstrates that the DEM model is able to capture how the moment due to friction influences the normal velocity of the contact patch and hence the normal overlap. Therefore, full coupling is taking place between all relevant first-order collision physics. In the FEA simulations, the self-servo effect was responsible for reductions in CoR_t as large as



(a) Normal coefficient of restitution CoR_n .



(b) Rebound angular velocity Ω .

Fig. 23 DEM predictions of non-spherical combined primary and secondary particle rebound vs. FEA from [20]. Particles are 5 mm diameter equivalent alumina ellipsoids impacting an aluminium substrate with $\theta_i = 45^\circ$ for the primary impact.

24%, from 0.91 to 0.69. Note that here where $\text{CoR}_n = 0$, the particle centroid is still moving towards the wall after the first rebound.

The collisions simulated at $\theta_i = 45^\circ$ involve plastic deformation, as demonstrated by the reduced CoR_n in Figure 21(a) compared to Figure 20(a). The added complexity of modelling plastic deformation leads to a small reduction in accuracy between $\theta = -30^\circ$ and $\theta = -90^\circ$, shown by Figures 21(b) and 21(c). However, the DEM model is still able to broadly match the FEA predictions across all orientation angles. The DEM approach models the collision until detachment from the surface. For an additional collision to occur it is only necessary that the particle angular velocity is sufficient to bring a point on the spheroid back into contact with the surface. This is also a function of aspect ratio, initial impact position and outbound velocity vector. Therefore, the normal, tangential and angular velocities of the spheroids following their first collision are held constant and an explicit time-stepping scheme is used to predict whether additional collisions occur. It displaces a 2D representation of the spheroid from the point of first rebound to the point where the particle either re-collides or is sufficiently far away from the surface. It is also able to predict at what orientation angle it re-collides with the surface, if applicable. A timestep sensitivity study confirmed that $O(10^3)$ timesteps adequately resolved particle dynamics. This is the same approach taken by the authors in [20]. The rebound velocities from the first collision plus the new orientation angle are

used as inputs to a new DEM simulation. This process continues as many times as is necessary for the particle to either rebound or stick to the surface. In the present simulations, no more than two bounces occurred per collision event.

The effects of secondary impacts are shown in Figure 23, where the DEM model again produces accurate predictions of particle rebound compared to FEA. The collisions shown are for an initial impingement angle of $\theta_i = 45^\circ$, as the substantial computational cost of the FEA simulations prevented second bounce simulations for both impingement angles. Note that, due to the small effect of secondary collisions on tangential rebound, a plot of CoR_t is omitted for brevity. The CoR_n is given with respect to the initial impact velocities, hence show the overall “collision event”. Regions with significant plastic deformation show the greatest deviation from experiment, likely due to the compounding errors from two consecutive simulations, however the boundaries between regions of primary and secondary collisions appear well defined by the time-stepping scheme. The step-change in rebound characteristics with the second bounce, combined with the large gradients, demonstrate the importance of including multiple bounces in rebound modelling. The results shown in Figure 23 have the additional benefit of validating the ability of the DEM model to predict collisions with substantial incoming angular velocities, with up to $|\Omega| = 1500 \text{ rad s}^{-1}$ as shown by Figure 21(c).

CONCLUSIONS

A model has been presented that can predict the rebound trajectory and angular velocity of spherical and non-spherical particles considering inelastic, viscoelastic and adhesive behaviour. These represent all relevant first-order physical phenomena for the rebound of particulates in gas turbine secondary air systems. Predictions were accurate when compared to experimental data across a range of particle diameters, velocities and impingement angles applicable to gas turbine components. The model is largely deterministic, directly simulating the relevant collision physics that occur throughout the contact time and hence can be used almost entirely with published materials properties. External effects like temperature and surface roughness can be included through augmented input parameters, while the effects of squeeze-film damping and rolling adhesion were found to be negligible for cases applicable to gas turbines.

Previous work by the authors has shown the importance of collision-induced rotation and coefficients of restitution on rebound trajectory and deposition. In particular, the qualitative distribution of deposition predicted by CFD was highly sensitive to rebound characteristics. The first inclusion and validation of non-sphericity in a deterministic manner will allow far superior predictions of particle transport where many repeated collisions occur, as is known to be the case in the secondary air system. Model predictions compare favourably with existing energy-based methods which fail to capture the underlying collision physics. The inclusion of viscoelastic dissipation in particular is shown to remove a dependency of yield stress on non-physical parameters. However, fitting the viscoelastic dissipation coefficient proposed to experimental results suggests that this may itself integrate a number of physical phenomena and further work is required to reduce dependency on empirical data. The force-based, explicit nature of the DEM also presents a flexible and adaptable platform for the inclusion of further physical phenomena.

The accompanying second part to this paper will demonstrate how to apply the DEM-based non-spherical bounce stick model to CFD, considering surface roughness. The spherical, smooth-wall version of the model has previously been shown to provide good predictions of deposition distribution. Hence, the developments described here are expected to significantly improve CFD predictions of deposition in gas turbine components.

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Statement of Authorship for joint/multi-authored papers for PGR thesis

To appear at the end of each thesis chapter submitted as an article/paper

The statement shall describe the candidate's and co-authors' independent research contributions in the thesis publications. For each publication there should exist a complete statement that is to be filled out and signed by the candidate and supervisor (**only required where there isn't already a statement of contribution within the paper itself**).

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Student Confirmation

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Supervisor Confirmation

By signing the Statement of Authorship, you are certifying that the candidate made a substantial contribution to the publication, and that the description described above is accurate.

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Supervisor comments: The motivation for the research was prompted from the overall research aims of the group. Profs. Gillespie and McGilvray supervised the research and identified the overarching research strategy.			
Signature		Date	23/8/2022

6 Modelling Particulate Deposition in Gas Turbines Part II: Prediction and Validation of Deposition Distributions

Predicting the spatial distribution of deposition in a system requires accurate particle tracking and predictions of particle-wall interaction. As demonstrated in Chapter 3, how particles rebound will affect the flowfield they experience and hence the likelihood of downstream deposition. Both the CRW turbulent transport model described in Chapter 2.4 and the bounce stick model developed in Chapter 5 have been shown to be accurate when compared to experimental data. Combining the two models therefore presents the opportunity to test the ability of CFD to predict deposition.

The following paper is based on a conference publication from the 2022 ASME Turbo Expo. It forms the second part of a two-part submission to the Journal of Turbomachinery, describing a robust methodology for the prediction of deposition in gas turbine components. The CRW and DEM models were combined in CFD simulations of flow through an S-bend with micron-scale particles of ARD at an elevated temperature. The results of the simulations were compared with existing experimental data collected at Oxford, presenting the first experimentally-validated predictions of deposition distribution in the open literature for complex flows. The results demonstrate the importance of an accurate bounce stick model, with other energy-based models failing to capture the deposition trend. The agreement with experimental results achieves the primary aim of this DPhil research: to develop a bounce stick model for the deposition and rebound of particulates in gas turbine components.

The original paper has been extended to include surface roughness and the modelling of non-spherical particle impacts in CFD. Whilst the model presented in the previous chapter can accurately model the rebound of spheroids, it requires the particle orientation and angular velocity at impact. These are coupled to the fluid solution, necessitating the use of CFD. Where the scale of surface roughness is much greater than the diameter of the particle, it acts only to augment the angle of incidence. Therefore, surface roughness modelling is extraneous to the fundamental collision physics discussed in Chapter 5 and included here instead.

The author of this thesis is the primary author of the paper. Nikul Vadgama produced the flow solutions and set up the particle injections in ANSYS Fluent while also a DPhil candidate at Oxford. The author then used this set-up to run the DEM-based simulations that form the central contribution to knowledge in this work. Florian Villain, currently a DPhil candidate at the OTI, helped optimise and port an earlier version of the DEM MATLAB code to a C-based Fluent UDF. Simon Beal collected the experimental data as part of his fourth year undergraduate project at the OTI while Professors McGilvray and Gillespie supervised the research. Benjamin Littlely of Rolls-Royce provided invaluable feedback and advice on the model development as part of the MALIT program.

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DRAFT Modelling Particulate Deposition in Gas Turbines Part II: Prediction and Validation of Deposition Distributions

Cooling passages and the secondary air system of gas turbine components are prone to blockage from sand, dust and ash. The ability to model deposition of non-spherical particles accurately using CFD would allow the prediction of in-service performance degradation and the design of deposition-tolerant hardware. Predictions of deposition require accurate modelling of particle transport and wall interactions. Bounce stick models predict whether a particle will bounce, stick, or shatter upon impact and calculate rebound trajectories. Turbulent transport models allow the interaction of particles with near-wall turbulent structures to be predicted in RANS CFD solutions. This paper implements a Continuous Random Walk (CRW) transport model with a Discrete Elements Methods (DEM) based bounce stick model, described previously, to predict deposition in commercial CFD software. These are the first such simulations in the open literature to incorporate particle shape and surface roughness. The resulting spatial trends of deposition are compared with experimental data of particle deposition in an S-bend. The case considered is representative of the flow and metal conditions, particle size and loading distribution, and passage geometry seen in high pressure turbine blade cooling passages. Numerical predictions of deposition distribution show good qualitative agreement with experimental data. This validates the combined CRW/DEM approach for modelling the distribution of particulate deposition in gas turbine components. The approach is therefore suitable to assess and compare the susceptibility of components to particulate damage in industry. To the author's knowledge, this is the first example in the open literature of experimental comparison of deposition trends in CFD. The approach provided reasonable first-order estimations of quantitative deposition heights, which may be used to estimate component-level performance degradation in-engine. The deposition heights and integral mass fractions predicted were approximately two-thirds of those from experiments, throughout the domain. More accurate quantitative predictions of deposition will require a suitable deposit evolution and erosion model and improved material data, which is not yet available in the open literature. The inclusion of the Magnus force altered quantitative and qualitative measures of deposition throughout the domain, demonstrating the importance of modelling collision-induced rotation in particle tracking. The performance of the DEM bounce stick model was favourable compared to energy-based alternatives which showed reduced accuracy in inertia-dominated regimes where multiple bounces occurred per particle. On average, approximately eight impacts were observed per particle, reinforcing the dual importance of accurate bounce stick and turbulent transport models.

Keywords: Particulate Deposition, Gas Turbines, Bounce Stick Models, Non-Spherical, Surface Roughness.

NOMENCLATURE

Abbreviations

ARD	Arizona Road Dust
CIR	Collision-Induced Rotation
CRW	Continuous Random Walk
CV	Critical Velocity bounce stick model, [1]
DEM	Discrete Element Methods
DRW	Discrete Random Walk
OSU	Ohio State University bounce stick model, [2]
RSM	Reynolds Stress Model
UDF	ANSYS Fluent User Defined Function

Roman Symbols

$\dot{m}_{g,tot}$	Total gas mass flow, $g\ s^{-1}$
e_0	Viscoelasticity parameter for the DEM model, CoR_n with only viscoelasticity [3]
A_{proj}	Particle projected area, m^2
c_p	Particle specific heat, $J\ (kg\ K)^{-1}$
D_h	Passage hydraulic diameter, m
D_p	Particle diameter, μm
E	Elastic modulus, Pa
G	Shear modulus, Pa
k_p	Particle thermal conductivity, $(m\ K)^{-1}$
L_{proj}	Particle projected length, m
M_{reb}	Rebound moment for non-spherical particles, Nm
s	Spread of raised cosine distribution, $^\circ$

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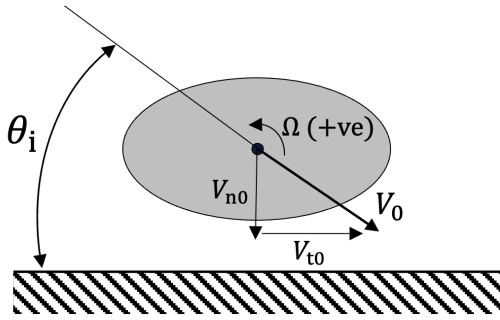


Fig. 1 Particle sign convention.

Greek Symbols

γ	Surface free energy, J m^{-2}
Ω	Particle rebound angular velocity, rad s^{-1}
ϕ	Surface roughness angle, $^\circ$
ρ_p	Particle density, kg m^{-3}
σ	Standard deviation of surface roughness angles, $^\circ$
σ_y	Yield stress, Pa
θ	Particle orientation angle w.r.t. the surface, $^\circ$
$\theta_{i,\text{eff}}$	Effective particle impingement angle accounting for surface roughness, $^\circ$

Non-Dimensional Parameters

CoR_n	Normal Coefficient of Restitution $\left[\text{abs} \left(\frac{V_{n3}}{V_{n0}} \right) \right]$
CoR_t	Tangential Coefficient of Restitution $\frac{V_{t3}}{V_{t0}}$
μ	Coefficient of friction
R_0	S-bend radius of curvature, $2R_{\text{bend}}/D_h$
D	Normalised distance for spatial convergence criteria
$M_{1,2}$	2D mass fraction deposition distributions for spatial convergence criteria
AR	Particle aspect ratio $\frac{\pi L_{\text{proj}}^2}{4A_{\text{proj}}}$

INTRODUCTION

The ingestion and deposition of atmospheric particulates are known to cause significant damage to gas turbine components. Coupled erosive, corrosive and geometry-altering deposition effects risk the failure of hot gas path components and a decrease of the operating surge margin [4]. Mass deposition events like the 1982 Galunggung BA009 volcanic ash exposure garner significant press attention, although a less publicised threat posed by atmospheric contaminants is the long term degradation of the jet engine. Second-order damage mechanisms arising from reduced cooling efficiency and corrosion have further deleterious effects on efficiency, safety and operating costs throughout fleet service life. Notably, the longevity of turbine blades is known to be affected by corrosion-fatigue from deposition in the secondary air system [5, 6]. As the complete filtration of intake air is unfeasible, the ability to accurately model deposition is essential to design particulate-tolerant hardware and predict the cost of ownership effects that arise from the ingestion of atmospheric contaminants.

Particle deposition modelling in CFD can be divided into three fundamental stages: transport modelling, accounting for fluid effects and turbulence on particle motion; bounce stick modelling, predicting particle-wall interactions; and deposit evolution modelling, concerning agglomeration and erosion of particles on the wall. Typically, a Lagrangian approach is used to model the discrete phase with tracking and bounce stick behaviour modelled independently, as in [7–9]. The present study presents a methodology for modelling deposition in the secondary air system of gas turbines. As the compressor exit temperature is likely to be below the softening temperature of ingested particulates, approx-

imately 1000°C [10–12], it is likely that particles will bounce multiple times before depositing. Previous work by the authors has shown that how particles rebound affects the likelihood and location of downstream deposition through exposure to different flowfields and Collision-Induced Rotation (CIR) [13]. Hence, accurately modelling deposition in the secondary air system will require validated models of turbulent transport and bounce-stick behaviour. The authors have previously presented a Continuous Random Walk (CRW) model of turbulent transport and a Discrete Element Methods (DEM) based bounce stick model, validating both independently with experimental data. These models, discussed below, have shown significant improvements over similar approaches in the open literature.

However, deposit evolution and erosion modelling is less mature. Bowen and Bons [8] present an experimentally-validated method for deposition predictions with conjugate mesh morphing, but considers particle diameters $< 6\mu\text{m}$ and so excludes erosive effects. The larger particles studied here ($> 20\mu\text{m}$) are likely to cause erosion, as demonstrated by the experimental results from Libertowski et al. [14]. While Libertowski et al. present a methodology for erosion modelling, substantial fitting to experimental data is required. It is also coupled to the OSU bounce stick model, the limitations of which for the present simulations are discussed below. The model presented by Casari et al. [15] takes a similarly empirical approach to erosion, coupled to a stochastic particle sticking model. This contrasts with the largely deterministic approach taken by the DEM-based method used in the present work. Therefore, the following simulations exclude deposition evolution and erosion. This allows the experimental validation of the coupled CRW/DEM approach for prediction of qualitative deposition trends, independently of uncertainty from other empirical models. Further work by the authors will develop a model, validated by experimental data, that is suitable for use with the DEM-based approach described herein.

This CRW/DEM approach is applied to CFD simulations of flow through a double S-bend. The simulations are representative of flow conditions, geometry and temperatures in a secondary air system cooling passage. The methodology presented here also allows for the inclusion of surface roughness and the collisions of non-spherical particles. Numerical distributions of deposition height are compared to experimental values from [16]. Given the exclusion of deposit evolution modelling, these results provide first-order estimates of the location and quantity of deposition. This represents, to the authors' knowledge, the first experimentally-validated predictions of spatial deposition distributions for Lagrangian particle tracking simulations. This approach allows the comparison of geometries for their susceptibility to particulate damage and the identification of likely points of failure. Hence, a robust methodology is presented for the simulation of deposition in gas turbine components, for use in commercial CFD solvers by academia and industry to develop deposition-tolerant hardware.

Turbulent Transport Models. Turbophoresis is the phenomenon that causes particles to migrate from regions of high turbulence to regions of low turbulence [17]. The difference in turbulent dispersion rates between these regions causes particles to accumulate preferentially in the viscous sublayer and buffer region, due to the sharp gradients of turbulence intensity near the wall. Particle interaction with near-wall coherent structures like streamwise vortices, ejections and in-sweeps increase deposition, on average, however the process is necessarily stochastic. Considering turbophoretic effects, three regimes of deposition exist: diffusional, diffusion-impaction and inertia-moderated [18]. Particle impaction in the diffusional regime is governed by Brownian motion, where non-dimensional deposition decreases with particle diameter. For slightly larger particles in the diffusion-impaction regime, turbulent eddies impart energy to the particle which leads to a significant increase in deposition with particle inertia. In

the inertia-moderated regime, for relatively large particles, the increasing inertia of the particles relative to force imparted by eddies reduces the influence of turbulence on particle motion.

Particles in the gas turbine secondary air system are generally in the diffusion-impaction regime [19], hence require a turbulent transport model with RANS to approximate the instantaneous fluctuating velocities experienced by each particle. Two models popularly used are the Discrete Random Walk (DRW) and the Continuous Random Walk (CRW). The DRW assumes that the velocity fluctuation experienced by a particle is constant over the length of an eddy, derived from a Gaussian random distribution. The CRW models the unsteady velocity experienced by a particle during its instantaneous interaction with flow eddies. It largely eliminates the order of magnitude overprediction of deposition by the DRW for particles in the diffusion-impaction regime [20, 21]. However, acquiring the necessary turbulent statistics to apply the CRW from RANS flow solutions is challenging, the CRW having been developed using DNS. This necessarily limited the initial application of the CRW to simple flows. Recent developments have allowed anisotropic flow properties and an appropriate time step to be determined on a cell by cell basis using RANS or uRANS solutions employing a Reynolds Stress turbulence Model (RSM) [16, 22]. This allows the CRW to be applied to more complex flow geometries such as those described below. This paper provides the first results of such a strategy.

Bounce Stick Modelling. Bounce stick models predict the rebound trajectories of particles from a wall through three parameters: angular velocity Ω , and the normal and tangential Coefficients of Restitution (CoR):

$$\text{CoR}_n = \left| \frac{V_{n3}}{V_{n0}} \right| \quad (1)$$

$$\text{CoR}_t = \frac{V_{t3}}{V_{t0}} \quad (2)$$

where the subscripts n and t denote wall-normal and wall-tangential respectively (see Figure 1) and 0 and 3 denote prior to and following the collision. Sticking is defined where $\text{CoR}_n = 0$. The approach to bounce stick modelling varies widely in the open literature with most models fitting at least some model parameters to empirical data. The Energy-Based Fouling Model for Gas Turbines (EBFOG [15]) presents an empirical approach, where particle energy at impact is related to a sticking probability. Increased energy flux normal to the surface, including the thermal energy of the particle, will increase the likelihood of deposition. This assumption fails to capture observed [23] low velocity deposition of small particles due to van der Waals adhesion and does not predict rebound trajectories. It is therefore particularly unsuitable for use in the secondary air system where particles may deposit below their softening temperature. Another empirical approach by Senior and Srinivasachar [24] and refined by [25] expresses the change in particle mechanical properties with temperature through viscosity. The Critical Viscosity model estimates a sticking probability based on temperature, calibrated to experimental data. Where extensive data for fitting is available *a priori*, it provides a simple and accurate model for sticking but necessarily neglects rebound property predictions. A largely deterministic approach was proposed by Singh and Tafti [26], and refined in [27, 28]. The latest iteration presented the most comprehensive overview of collision physics at the point of publication, including viscoelastic deformation and the effects of surface roughness on adhesion and plastic deformation. Fitting to empirical data was employed to allow predictions of tangential rebound and angular velocity, however experimental validation

was limited to total CoR, neglecting individual validation of normal and tangential modelling. Therefore, further validation is needed before use in CFD.

The OSU deposition model [2] presents an energy-based, semi-empirical approach that was validated separately for normal and tangential rebound. Predictions are accurate when multiple model parameters are fitted to experimental data, notably the yield stress σ_y (which varies as a function of impact velocity to account for strain rate effects [29]) and surface free energy γ for adhesion. Previously, Gaskell et al. [3] found, unsurprisingly, that OSU model predictions of CoR_n and CoR_t failed to match experimental data if constant values of σ_y and γ available from literature were employed, making it difficult to use without empirical tuning. The model also neglects to model Ω , preventing the inclusion of CIR in deposition modelling. The Critical Velocity (CV) model [1] presents the most physics-based approach of the energy-based models, using the widely implemented JKR adhesion model and an empirical strain rate term to produce accurate predictions of CoR_n and CoR_t at low normal velocities [3]. However, its inability to account for plastic deformation, tangential compliance of the contact patch during highly normal collisions, and angular velocity presents serious limitations to its use in gas-turbine representative systems.

The accompanying first part to this paper describes a DEM-based bounce stick model proposed by the authors to address the limitations of energy-based and largely empirical methods. The explicit, force-based approach incorporates all relevant physical phenomena from existing literature, namely: plastic deformation, van der Waals adhesion, viscoelasticity, friction, non-sphericity and squeeze-film damping. Predictions of rebound characteristics CoR_n , CoR_t and Ω were validated against experimental data and FEA simulations, and showed significant quantitative improvements in accuracy over the OSU and CV models. DEM models were originally developed for geotechnical simulations [30] and are still most frequently used for the simulations of granular flows e.g. in grain silos [31]. Existing DEM-based collision models may not necessarily include all the physical phenomena relevant to the secondary air system (an example being the built-in DEM collision model from ANSYS Fluent [32]). The authors' implementation is designed to be computationally efficient, acting from the point of first contact with a wall to the point of rebound, allowing the simulation of systems with $O(10^6)$ particles. Environmental factors such as changing temperature are accounted for by modifying the material parameters that are input to the model, e.g. temperature dependent correlations of the elastic modulus. Surface roughness can be accounted for by stochastically augmenting the particle angle of incidence, as described later. The force-based nature of the model allows the straightforward inclusion of additional physical phenomena, notably particle non-sphericity which has been shown by the authors to significantly alter how a particle rebounds [33]. The present work explains how to implement the DEM model in CFD, predicting particle orientations and angular velocities at the point of impact. Modelling the collision deterministically is crucial, as statistical distributions of particle rebound from impinging jets may be biased by particle preferential orientation, as discussed later. The particle velocity is calculated at each collision time step by integrating the equations of motion:

$$m \frac{d\vec{V}}{dt} = \begin{bmatrix} m \frac{dV_t}{dt} \\ m \frac{dV_n}{dt} \\ 0 \end{bmatrix} = \begin{bmatrix} F_t \\ F_n + F_{nd} \\ 0 \end{bmatrix} \quad (3)$$

$$I \frac{d\Omega}{dt} = M_t + M_r + M_{\text{reb}} \quad (4)$$

where F_f is the frictional force that acts tangentially on the contact patch from [30], F_n is the normal force between the wall and contact patch (including adhesion, plastic and elastic deformation) [34] and F_{nd} is the normal dissipative force resulting from viscoelastic deformation [35]. The sub-model for F_n , with the most influence on particle adhesion and rebound, is derived from Hertzian collision physics, the widely used JKR model of adhesion [36] and perfectly plastic behaviour described by Davies [37]. Moment M_f results from the frictional force F_f acting about the particle centroid while M_r is the contribution of rolling adhesion to particle motion [38]. The rebound moment M_{reb} is the product of the normal contact force and any horizontal displacement between the contact patch and centre of mass of the particle, where the particle is not spherical. The only empirical input to the model is the viscoelasticity parameter e_0 , the CoR_n where only viscoelasticity affects normal rebound. This can be estimated from low-velocity single particle collision data like [23, 29, 39], where the normal velocity is high enough to overcome adhesion but lower than the plastic yield velocity. The particle is defined as stuck where its centroid oscillates about equilibrium.

Non-Spherical Particle Transport. Previous work by the authors [33] describes significant differences between the collision physics of spherical and non-spherical particles. Normal coefficients of restitution CoR_n were up to 84% lower than an equivalent sphere, with the rebound angular velocity Ω varying in both sign and magnitude. Secondary impacts, where more than one point on the particle impacts the surface in a single collision, had highly non-linear effects on the rebound trajectories. The accompanying first part to this paper demonstrates a robust methodology to predict the rebound of non-spherical particles. However, the implementation of the model in CFD requires the further consideration of particle-fluid interaction.

Non-spherical particles in turbulence experience orientation-dependent forces and torques that are, themselves, dependent on shape, initial orientation, and fluid and particle inertia. Marchioli et al. [40] found through DNS that long fibres exhibited a higher wallward drift velocity in turbulent channel flow than spherical particles. In real systems, this is likely to increase deposition for non-spherical particles. This conclusion is echoed by many other workers in the literature [41–43]. Both prolate and oblate spheroids are also known to segregate into low speed streaks near the wall, with the degree of segregation increasing with particle inertia [44]. A turbulent transport model that is optimised for non-spherical particles is not used here, but will be developed in further work. For the purposes of the Lagrangian tracking performed, the particles are considered spherical. While version 19.2 of Fluent has functionality to consider non-spherical particles, its lack of orientation-dependence makes it an unsuitable choice for the simulations presented below, for the reasons presented in the remainder of this subsection.

Prolate spheroids, a ‘rugby ball’-type shape, are shown to exhibit preferential orientations in simple shear flow. A lattice Boltzmann method was used by Mao and Alexeev [45] to show that neutrally-buoyant particles drifted from an arbitrary initial orientation towards tumbling. Tumbling is the ‘end-over-end’ motion defined by the orthogonality of a particle’s angular velocity vector and its major axis. Shear flow is particularly relevant to deposition simulations, given its similarity to the viscous sublayer. Considering internal flow that is representative of the secondary air system, a typical characteristic height of 50 mm, velocity of 20 m s⁻¹ and density of 11 kg m⁻³ leads to a viscous sublayer that is an order of magnitude larger than the diameter of a micron-scale particle. A further DNS study by Zhao et al. [46] demonstrates that inertial prolate spheroids in turbulent channel flow show strong preference for tumbling at $y^+ \leq 15$.

The angular slip velocity of particles near the wall was studied by Marchioli et al. [47]. The RMS fluctuations of angular slip increase with non-sphericity, peaking below $y^+ = 10$. Actual slip velocities varied only by approximately 50% between particles with Stokes numbers $Stk = 1$ and $Stk = 100$. It can be shown analytically that tracer prolate spheroids in 2D Stokes flow have an angular velocity described by Equation 5, from [48]:

$$\Omega = \dot{\theta} = \frac{1}{AR^2 + 1} \left(\frac{1}{2} (AR^2 - 1) \sin(2\theta) \left(\frac{\delta u_y}{\delta y} - \frac{\delta u_x}{\delta x} \right) + (\sin^2(\theta) + AR^2 \cos^2(\theta)) \frac{\delta u_y}{\delta x} - (\cos^2(\theta) + AR^2 \sin^2(\theta)) \frac{\delta u_x}{\delta y} \right) \quad (5)$$

where θ is the orientation angle, AR is the particle aspect ratio and $\bar{u}$ is the fluid velocity vector. Note that AR is defined as the ratio of major to minor axis lengths. This describes a periodic angular velocity peaking where the major axis of the particle is orthogonal to the mean velocity vector. This appears to echo the findings of the DNS studies, including the tendency of the particle to align its major axis with the mean velocity vector. The DEM-based bounce stick model discussed previously can predict particle rebound, given its shape, initial velocity vector and orientation angle. The challenge of the present work is to predict a representative range of particle orientations and angular velocities as input to the model. How this is achieved using RANS CFD is described later.

EXPERIMENTAL SET-UP

Vadgama et al. [49] present an experimental study of the deposition of ultrafine Arizona Road Dust (ARD) in an S-bend geometry. The spatial distribution of deposition throughout the test-piece will be used to qualitatively validate the predictions of the combined CRW/DEM approach. The S-bend geometry produces complex flow features similar to cooling passages: notably contra-rotating Dean vortices that result from fluid experiencing centrifugal force and accelerating radially outwards. Crucially, the use of 90° bends as opposed to 180° bends ensures particles travel throughout the domain, not all adhering in the first bend. This produces a suitable validation dataset for bounce stick behaviour. Thermophoretic behaviour is matched with representative gas and wall temperatures (830 dec C and 1230 deg C respectively), while a similar Reynolds number ($Re = 3442$) ensures that turbophoretic effects are captured. A schematic of the rig is shown in Figure 2, where primary and secondary flow paths are fed from dry compressed air at 7 barg. The primary gas path is passed through an 8 kW electric heater, while the secondary gas path, at ambient temperature, supplies a particle dispersion device. A co-axial mixing chamber forms the inlet fluid stream for the test-piece, generating an isothermal uniformly-laden flow. The particle volume fraction was less than 1×10^{-7} in all experiments, ensuring one-way coupling between the solid and fluid phases. A summary of the experimental parameters used here are given in Table 1 while full details of the experimental set-up are provided in [49].

A schematic of the test-piece is shown in Figure 3. The inlet flow bifurcates, allowing two S-bend geometries to be tested simultaneously. The following numerical simulations focus on a single S-bend with non-dimensional radius of curvature $R_0 = 2R_{bend}/D_h = 10$, where R_{bend} is the bend radius and D_h the passage hydraulic diameter. This corresponds to Experiment 1 in [49]. The S-bend passage has a rectangular cross-section 9 mm × 3 mm (H × W), swept through two 90° bends before exiting the test article, diluted and passed through a HEPA filter. The test article sits within an oven, capable of heating the component to 1450 deg C. Machined

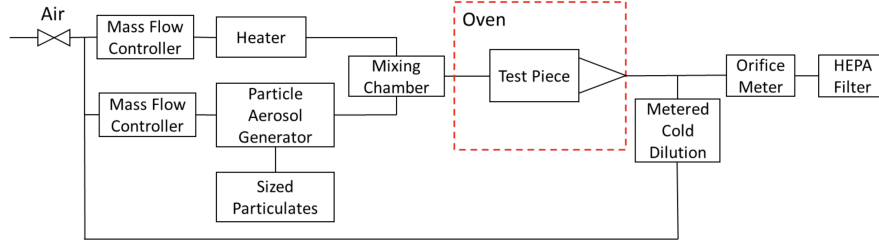


Fig. 2 Schematic of the air flow rig. Flow from left to right. Figure from [49].

Table 1 Experimental parameters.

Re	T_w (°C)	T_g (°C)	R_0	$\dot{m}_{g,tot}$ (g s ⁻¹)
3442	1239 ± 6.0	828 ± 4.2	10	1.6

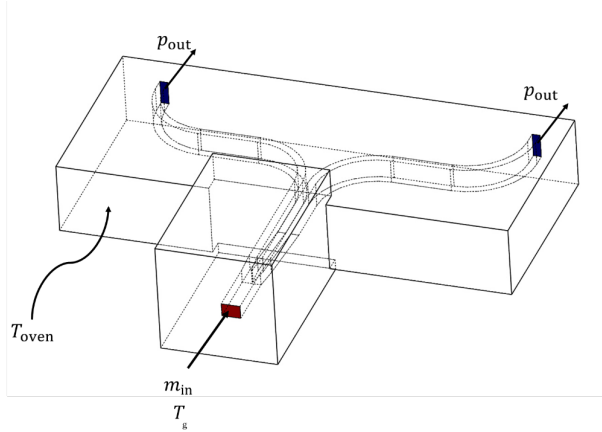


Fig. 3 Experimental test-piece and conjugate simulation domain. Figure from [50].

from stainless steel (SS316), the test article and its holder provided sufficient thermal mass for isothermal conditions throughout each 20 minute test. Each test article could be disassembled to allow maps of surface deposition to be created from an Alicona Infinite Focus microscope, with ± 10 nm vertical and ± 400 nm horizontal resolution.

FLUID PHASE

Set-Up and Solution. The numerical heat transfer simulations conducted were fully conjugate, i.e. the solid material and fluid domain were coupled. Figure 3 shows the domain and boundary conditions for all simulations. Note that only a single passage from Figure 3 was simulated using CFD for computational efficiency. The inlet mass flow rate and temperature are defined using the measurements from the experiment detailed in the previous subsection (Table 1). The outlet pressure is similarly matched to experimental measurements. In the conjugate analysis performed, use is made of the model's large thermal mass to set a steady isothermal external metal temperature. As per [16], a Reynolds Stress Model (RSM) with wall reflections was used for turbulence modelling. This was found to best predict the important anisotropic turbulent properties required for the CRW model. The simulations were solved using a SIMPLE (Semi-Implicit Method for Pressure Linked Equations) pressure-velocity coupling. Third-order MUSCL (Monotone Upstream-Centred Schemes for Conservation Laws) were used for the spatial discretisation as it has the potential to improve the spatial accuracy by reducing numerical diffusion in highly 3D flows such as these [32]. At convergence,

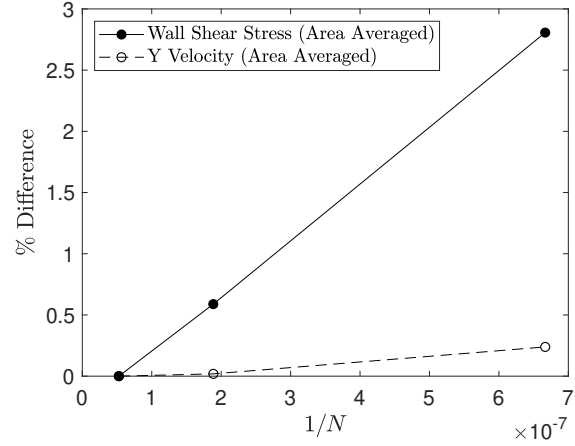


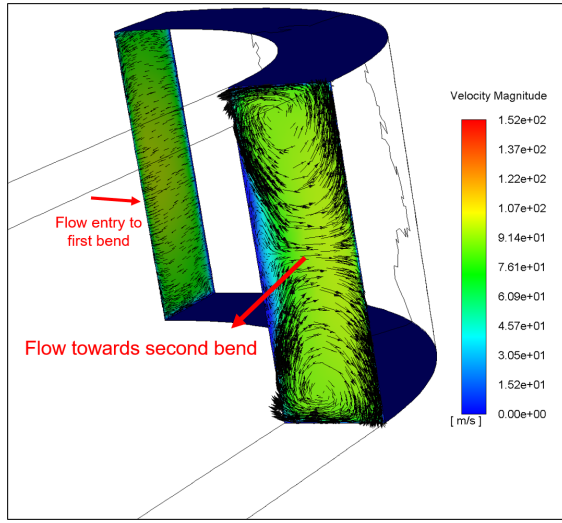
Fig. 4 The change in residuals of wall shear stress and exit plane axial velocity. The horizontal axis is the reciprocal of the total number of solid and fluid cells.

energy equation residuals were $\leq 10^{-7}$, continuity $\leq 10^{-9}$ and all others $\leq 10^{-5}$. The gas, lab air at 7 barg, was assumed to be an ideal gas that followed Sutherland's law. Gravity was turned on for all simulations unless explicitly otherwise indicated.

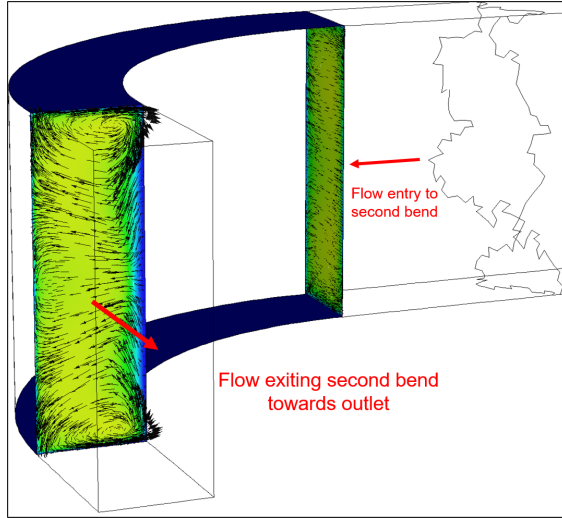
Mesh Sensitivity & Convergence. An unstructured grid was used for the simulations with an independence study used to confirm the suitability of the mesh. Three meshes were solved with 1.5×10^6 cells (0.9×10^6 fluid, 0.6×10^6 solid); 5.3×10^6 cells (3.3×10^6 fluid, 2.0×10^6 solid); and 19×10^6 cells (12×10^6 fluid, 7.0×10^6 solid). Two explicit fluid quantities were monitored to determine fluid phase convergence: tangential velocity at the exit (area averaged) and wall shear stress on the channel walls (area averaged). The first quantity was used as an indication of the fluid field's structure (i.e. the strength of the induced secondary flows). The second ensures the near wall fluid structure is converged which has been shown to be critical for accurate deposition predictions, and is directly used by the CRW model. Figure 4 shows that results of the medium density mesh fall within one percent of the high density mesh. This mesh was employed for all further work.

Fluid Phase Description. An understanding of the fluid phase is required in order to analyse the motion of particles. Here the key aspects of the fluid phase are discussed with respect to particle motion.

The primary drivers of motion of the fluid through the bend are the axial pressure gradient and bend curvature. As seen in 90° pipe flow, counter-rotating Dean vortices are induced as the fluid is accelerated around the bend. Figure 5 shows the formation of these vortices throughout the first and second bends, where the dual



(a) From bend 1 exit.



(b) From bend 2 exit.

Fig. 5 Contours of velocity around the first and second bends. Vectors showing tangential projections of velocity, demonstrating formation of Dean vortices. Arrows show flow direction. Colour scale is the same for both subfigures.

contra-rotating structure can clearly be seen through the velocity vectors on the exit plane of bend 1 in Figure 5(a). A region of separation is also visible on the inside of the bend. Figure 6 shows isocontours of helicity throughout the S-bend, where the Dean vortices persist throughout the channel connecting the first and second bends. The second bend in isolation would induce identical but counter-rotating Dean vortices to the first bend. Superposition of these two potential fields results in flow with complex secondary motion: corner vortices are visible in Figure 5(b).

DISCRETE PHASE METHODOLOGY

The particle trajectories are calculated using Fluent's inbuilt Lagrangian particle tracking tool with a user defined function (UDF) which implements the CRW (as described in [16]) and an in-built model for thermophoresis [20]. For computational efficiency, particle injection was limited to the uniform injection of particles into one leg of the flow domain (Figure 3) at the point of flow bifurcation. To replicate the particle distribution of the ultrafine ARD used in experiments, a Rosin-Rammler distribution with

10 discrete particle diameters was used. The distribution has a minimum of 9.7×10^{-7} m, a maximum 2.2×10^{-5} m, and a median of 5.2×10^{-6} m. The heat capacity and thermal conductivity of this dust is not well reported, but the dust is primarily quartz for which data are available and are used here [51]. Material properties were set to $\rho_p = 2649 \text{ kg m}^{-3}$, $c_p = 820 \text{ J (kg K)}^{-1}$, $k_p = 1.85 \text{ W (m K)}^{-1}$.

A key driver of this work is to determine spatially resolved maps of deposition. To allow this to be reliably predicted, the tracking has been conducted using the discrete phase convergence criteria developed in [19]. This determines the number of particles and injection sites necessary to achieve a representative result from this stochastic process. The key convergence metric is the normalised distance D shown in Equation 6, where M_1 and M_2 are 2D mass fraction distributions over the surface. Respectively, they refer to the deposition distribution before and after new data (e.g. another particle injection) is included.

$$D = \left(\frac{1}{2} \sum |M_1(x, y) - M_2(x, y)| \right) / \sum M_2(x, y) \quad (6)$$

The normalised distance D is reported at the highest number of particles injected/highest number of repeat injections. Thermophoresis and gravity were switched off for the convergence simulations to maximise possible variations due to turbophoresis. Thus the largest variation injection to injection should be observed and hence determine a sufficient injection methodology for all cases. The deposition on the bend walls can be discretised depending on the level of resolution required. In this case, 15 degree arc-wise and 1.5 mm high segments were used, creating a 6 by 6 grid over each surface. Figure 7(a) shows that at least 1×10^6 particles are required per injection. Figure 7(b) shows that if a single repetition of such an injection is made, this ensures that enough particle trajectories are sampled to give a representative distribution. In both Figure 7(a) and Figure 7(b) the inside of the second bend requires the largest number of particles to reach a converged solution. This is due to the limited deposition that occurs on this face, the importance of turbophoresis for this deposition to occur, and the limited remaining particles in the flow following deposition in the first bend.

The DEM-based bounce stick model [3], described in the Introduction, is implemented as a Fluent User Defined Function (UDF) and will be compared to the performance of the OSU and CV models. The DEM model was chosen due to its ability to model particle angular velocity Ω and superior accuracy in predictions of CoR_n and CoR_t throughout the full range of particle impingement angles and collision velocities expected. The particles simulated during collisions are prolate spheroids with an aspect ratio $\text{AR} = 1.9$, from the average of atmospheric micron scale particulates studied by [52]. Particles captured from the atmosphere may not be representative of those in the secondary air system, as larger particles in the compressor may break-up and be centrifuged away from the hub. However, the aspect ratio studied here is sufficient to demonstrate the underlying methodology. The Magnus force is calculated using correlations from Oesterlé and Dinh [53], the Fluent model most appropriate for this range of particle Reynolds numbers. Saffman lift is enabled in the solver while the pressure gradient and virtual mass forces are disabled, the particle density being substantially greater than the fluid density.

Obtaining accurate material properties with temperature dependence, particularly elastic constants, is a substantial challenge to bounce stick modelling. Other workers have fitted material properties to experimental data, notably [29]. To maintain independence from existing bounce stick models, the temperature-dependant material properties of quartz are used as it forms approximately 70% of ARD by mass [54]. Temperature-dependent correlations for

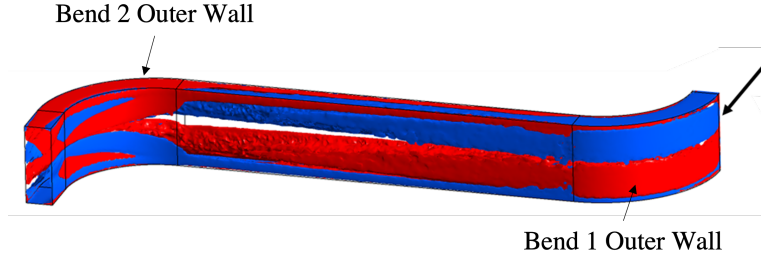
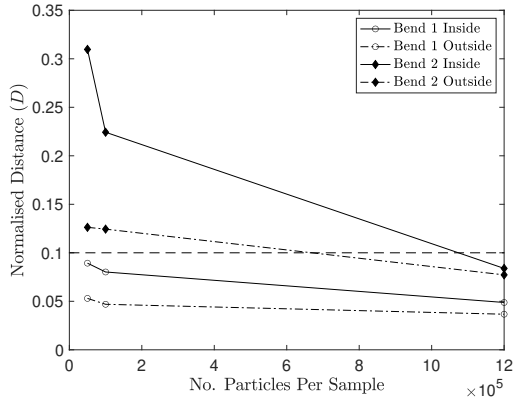
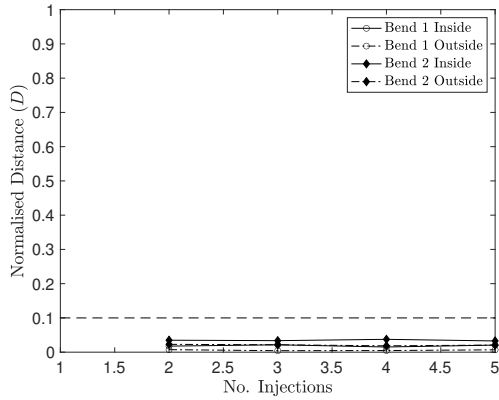


Fig. 6 Isocontours of helicity, at $\pm 180000 \text{ ms}^{-1}$. Arrow shows flow direction.



(a) Increasing the number of particles per sample (uniform spatial distribution, initially 2040 particles).



(b) Increasing the number of repeated sample injections whilst maintaining the same particle injection locations (uniform spatial distribution of 2040 particles).

Fig. 7 The normalised distance D , Equation 6, between distributions of mass fraction. A critical value of 10% (0.1) was chosen.

elastic constants and surface free energy were compiled by Covey-Crump [55] from [56–60] and used for all further simulations. Material properties are shown in Table 2, where temperature dependent values are calculated at each impact using the current cell temperature in the DEM Fluent UDF. It is assumed that the SS316 substrate will yield before the particles, hence the yield stress for SS316 is used as an input to the model. The viscoelasticity parameter e_0 , the CoR_n where only viscoelasticity affects rebound, is the only explicit empirical constant used in the DEM model. As discussed in the Introduction, it is set based on experimental rebound data. Viscoelasticity will decrease CoR_n with increasing

Table 2 Discrete Phase Material Properties. Temperature dependent properties compiled by Covey-Crump [55] from [56–60].

	ARD (Quartz)	SS316
E (Pa)	Temp. Correlation [55]	1.93×10^{11}
G (Pa)	Temp. Correlation [55]	4.23×10^{10}
σ_y (Pa)	-	216×10^6
ρ_p (kg m^{-3})	2649 [55]	-
γ (J m^{-2})	0.37 [55]	
μ	0.55 [2]	
e_0	0.90	

normal velocity, like plastic deformation. Adhesion, by contrast, has the most influence on particle motion at low velocities. Therefore, an appropriate estimation of e_0 is derived from the maximum CoR_n for a given dataset, generally at a high enough velocity for the effects of adhesion to be small while not sufficient for plastic deformation to occur. Reagle et al. [61] presents experimental rebound data for high temperature ARD. The highest CoR_n recorded is 0.8 at $\theta_i = 20^\circ$. As the CoR_n trends upwards with decreasing angle of incidence, e_0 was set to 0.90. This is supported by data from Whitaker and Bons [29], which shows a maximum CoR_n close to unity.

Surface Roughness. As previously discussed, surface roughness can be included in particle tracking simulations using the work of Sommerfeld and Huber [62]. This assumes that the scale of surface roughness is much greater than the diameter of the contact patch. By sampling the wall roughness of a component with an appropriate window distance, a statistical distribution of roughness angles can be produced. It is also assumed that this will be a normal distribution with a mean of zero, meaning that the roughness is isotropic across the surface. Care should be taken with this assumption if ‘saw-tooth’ type roughness results from manufacture. If the particle collision is normal to the surface, this distribution can be used directly to calculate the effective impingement angle of the particle in Equation 13. However, where the actual impingement angle of the particle θ_i is considerably less than 90° , the particle is far more likely to impinge on a roughness structure with positive inclination than one with negative inclination. This “shadow effect” can be seen by inspection of the geometry in Figure 8. This shifts the normal distribution of roughness angles to the right, making the effective angle of incidence $\theta_{i,\text{eff}}$ more normal. The PDF of the roughness angle distribution is given in Equation 7:

$$\text{PDF} = \frac{\sin(\theta_i + \tilde{\phi})}{\sin(\theta_i)} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\tilde{\phi}^2}{2\sigma^2}\right) \quad (7)$$

where $\tilde{\phi}$ is a set of roughness angles between -90° and $+90^\circ$, and σ is the standard deviation of the distribution. A normal distribution with standard deviation $\sigma = 10^\circ$ is shown in Figure 9 alongside its modified counterpart from Equation 7, where $\theta_i = 10^\circ$. Note

that the probability of impact drops to zero where $\phi \leq -\theta_i$. This is intuitively understood with reference to Figure 8 where, with sufficiently small θ_i , either particle would only impact the side of a roughness structure facing them, not any that face away. Using this PDF to calculate the effective angle of incidence could theoretically be achieved using inverse transform sampling, where the PDF is integrated to produce a CDF and inverted. What, before inversion, was the y-axis can then be sampled from a uniform distribution. However, the integral $\int e^{-x^2} dx$ has no closed form using standard functions. Therefore, a raised cosine distribution is used to approximate the PDF in Equation 7, shown in Equations 8 and 9.

$$\text{PDF}_{\cos} = \frac{\sin(\theta_i + \tilde{\phi})}{\sin(\theta_i)} \left[1 + \cos\left(-\frac{\pi\tilde{\phi}}{s}\right) \right] \quad (8)$$

$$s = \sqrt{\frac{\sigma^2}{\frac{1}{3} - \frac{2}{\pi^2}}} \quad (9)$$

The analytical PDF is compared to the cosine approximation in Figure 9, where good agreement is seen between the two. Equation 8 can then be integrated to provide an expression for the CDF, shown in Equation 10.

$$\text{CDF} = \frac{\csc(\theta_i)}{4s} \left[2\sin(\tilde{\phi})\sin(\theta_i) - 2\cos(\tilde{\phi})\cos(\theta_i) + \frac{s\cos\left(\tilde{\phi} + \theta_i - \frac{\pi\tilde{\phi}}{s}\right)}{\pi - s} - \frac{s\cos\left(\tilde{\phi} + \theta_i + \frac{\pi\tilde{\phi}}{s}\right)}{\pi + s} \right] \quad (10)$$

The CDF is bounded on the LHS by $\phi_{\min}$:

$$\phi_{\min} = \max \left\{ -\theta_i, -s \right\} \quad (11)$$

and on the RHS by $\phi_{\max}$:

$$\phi_{\max} = s. \quad (12)$$

By numerically inverting the CDF in Equation 10, a standard uniform probability distribution can be used to sample the modified PDF in Equation 8. The authors use a binary search method to considerably reduce the computational cost. The result of this is shown in Figure 9, where the histogram shows a good fit to both the cosine approximation and the analytical solution to the PDF. A randomly sampled surface roughness angle ϕ can then be used to calculate the effective angle of incidence $\theta_{i,\text{eff}}$ which is used as input to the DEM model. This allows conversion between the global frame of reference and that of the particle/roughness structure. Note that the rebound velocity vector must similarly be rotated by ϕ .

$$\theta_{i,\text{eff}} = \theta_i + \phi \quad (13)$$

Modelling Non-Spherical Collisions. To model the collisions of spheroids, the DEM bounce stick code requires the angular velocity and orientation of the particle at impact. As previously discussed, prolate spheroids show a strong preference for tumbling near the wall. Therefore, it is assumed that the particle will always tumble at the point of impact, meaning its average velocity vector lies in the same plane as its major axis (see Figure 10). Equation 5 provides an analytical solution to the angular velocity of a tracer spheroid in 2D Stokes flow, as a function of aspect ratio, orientation angle

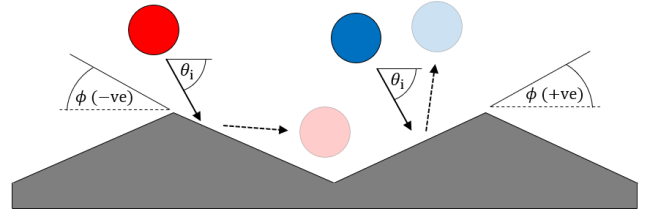


Fig. 8 Particles impinging on roughness structures with a positive (•) and negative (•) inclination angle ϕ .

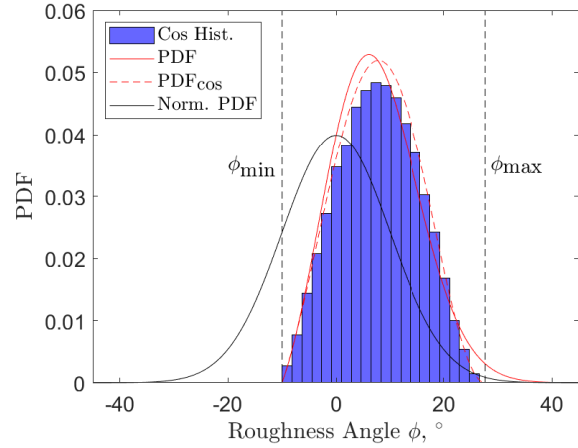


Fig. 9 Probability Distribution Function (PDF) showing roughness angles ϕ where $\theta_i = 10^\circ$. The roughness standard deviation $\sigma = 10^\circ$. Shown are the modified normal distribution from [62], the raised cosine approximation and an unmodified normal distribution. The histogram shows the result of randomly sampling the cosine approximation CDF in Equation 10.

and fluid shear. As discussed earlier, the absolute values and RMS fluctuations of angular slip velocities were not dissimilar between tracer and inertial spheroids. Therefore, Equation 5 is taken to be a reasonable approximation of Ω near the wall. Assuming that the particle is in simple shear flow, Equation 5 can be simplified to the form shown in Equation 14 based on the velocity gradient in Figure 10.

$$\Omega = \dot{\theta} = \frac{-1}{AR^2 + 1} \left[\frac{\delta u_x}{\delta y} \left(\cos^2(\theta) + AR^2 \sin^2(\theta) \right) \right] \quad (14)$$

By inspection, this is a non-linear ODE: we must know the orientation to know its rate of change, the angular velocity. The orientation, hence angular velocity, at impact will be random. However, we know that the particle will spend more time with its major axis parallel to the ground than perpendicular. Therefore, a uniform sampling of orientation angles, fed into Equation 14, will not be representative of the actual particle impacts. The orientation must be sampled in the time domain, which requires that the orientation is known at an arbitrary point in time. Equation 14 is therefore integrated numerically to provide the particle orientation throughout a full rotation. A random orientation is then sampled and used to calculate the angular velocity. This is illustrated by Figure 11, which shows the angular velocity and proportion of the rotation period spent at a range of orientation angles. These assume an aspect ratio $AR = 1.9$. The particle spends approximately $3.5\times$ longer with its major axis parallel to the ground ($|\theta| = 180^\circ$) than at right angles. For particle tracking simulations, the fluid shear $\delta u_x / \delta y$ is taken from the fluid solution.

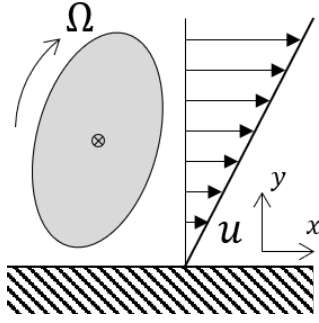


Fig. 10 A prolate spheroid ‘tumbling’ in simple shear flow near the wall.

The DEM collision model terminates when the contact patch detaches from the surface. However, this does not necessarily mean that the particle will rebound from the surface as secondary collisions are still possible. Indeed, with sufficient angular velocity, the contact patch may be moving away from the surface whilst the particle’s centre of mass may still be moving towards it. In this case, another point on the particle re-colliding with the surface is inevitable. Given that the particle will remain within a diameter’s distance to the surface, it is not feasible to pass the particle back to the tracking model to determine at what orientation it will re-collide. With FEA, the authors have previously used a time-stepping solution outside the collision model [33]. A point cloud that forms a 2D representation of the particle is displaced using the linear and angular rebound velocities until it either re-collides with the surface or escapes. In the event of re-collision, the new orientation angle is fed back into the collision model and the cycle is repeated until rebound or deposition. Fluid effects are neglected as the timescale for the re-collision of micron-scale particle is $O(10^{-7} \text{ s})$, based on an average angular velocity magnitude $|\bar{\Omega}| \approx 5 \cdot 10^6$. A similar method is employed here, instead representing the bounding ellipse of the particle and ground plane parametrically for computational efficiency. The ellipse is stationary with its centre at the origin, about which a line that represents the ground plane is rotated and displaced by the rebound linear and angular velocities. The intersection between an ellipse and straight line is described by a quadratic equation. Hence, where the discriminant of that equation is greater than or equal to zero, a secondary collision has occurred. A sensitivity study confirms that 10^3 timesteps is sufficient to resolve particle motion, where the timestep is defined by the particle angular velocity. The parametric version of the scheme has negligible computational cost in comparison to the DEM model. Hence, the only additional cost in simulating non-spherical particles arises from the need to simulate multiple collisions.

RESULTS

In this section the outcome of particle tracking simulations performed in Fluent using 1.3×10^6 particles spread over ten injections are reported. As the experimental roughness angle distribution is not known, simulations for a range of values of σ are performed first. These use spherical particles to isolate the effects of surface roughness from non-sphericity. Results are then presented for non-spherical particles with surface roughness, which are compared to state-of-the-art energy-based bounce stick models from the literature. The influence of collision-induced rotation is also investigated, through an additional simulation where the Magnus force on particles is disabled. Predictions of spatial deposition distribution are reported for the converged 6×6 grid that forms the outer wall of each bend. Deposition is presented as deposit height to allow comparison with experimental data. The effective material

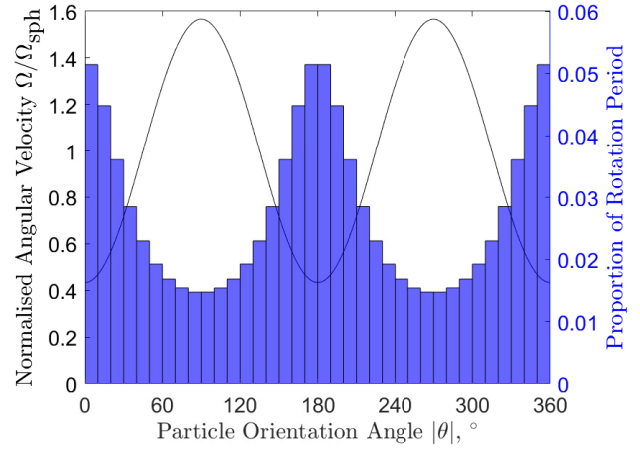


Fig. 11 Normalised angular velocity of an AR = 1.9 prolate spheroid, as a function of orientation. Also shown is the proportion of the rotation period spent at different orientations.

density of ARD was taken as 408 kg m^{-3} , accounting for packing porosity. This is based on a packing factor $PF = 0.18$ for a 1300 K impinging jet [63]. The total mass deposited in the simulation is scaled to match the total mass injected in the experimental case. This provides a qualitative and quantitative representation of how deposition is distributed throughout the domain. However, caution should be taken when interpreting quantitative predictions of deposition without a suitable deposit evolution and erosion model. The results presented here can be compared with prior work of the authors which exclusively simulated spherical particles impacting a smooth wall [64].

Note that the region of interest is labelled by the angular position relative to the centre of the bend (i.e. $\pm 45^\circ$ around each bend). Negative angles are on the upstream side of the bend, positive angles downstream.

Spheres with Surface Roughness. Four simulations of spheres were run with non-zero values of surface roughness angle ϕ . The standard deviation of the roughness distribution was set to $\sigma = [2.5^\circ, 5.0^\circ, 7.5^\circ, 10^\circ]$, providing an augmented effective angle of incidence $\theta_{i, \text{eff}}$ to the DEM model as described previously. The outbound velocity vector was also rotated by ϕ to account for the modified local surface geometry. The range of surface roughness distributions were chosen to reflect a likely range for the s-bend geometry, which was not profiled experimentally. Modified impingement angles compared to the smooth wall case will not only change the outcome of individual collisions, but will also alter whole-system deposition by changing the distribution of particles throughout the domain.

Figure 12 shows a histogram of the surface roughness angles encountered by particles throughout the domain for the $\sigma = 5^\circ$ case. The shadow effect, discussed previously, means that the distribution of roughness angles encountered by particles will depend on the actual impingement angle θ_i , hence cannot be known *a priori*. As expected, the particles were most likely to encounter a surface roughness structure with a positive inclination angle, a mean of 5.03° . The left-hand tail of the distribution suggests a small minority of near-normal impacts. This is confirmed by Figure 13, which shows the statistical distribution of effective impingement angles for different values of σ . As expected, the collisions are, on average, more normal with increasing surface roughness. Indeed only a small proportion of the collisions are near-normal with 0.2% above 45° . The average effective

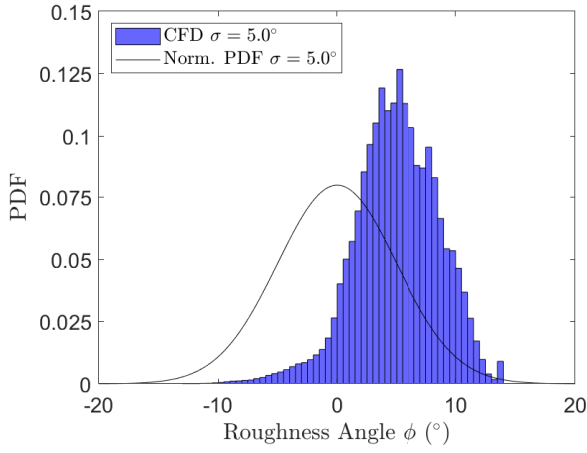


Fig. 12 Probability distribution of surface roughness angles ϕ , from CFD simulations with a standard deviation of surface roughness angles $\sigma = 5.0^\circ$.

impingement angle was $\theta_{i,\text{eff}} = 8.1^\circ$, compared to $\theta_{i,\text{eff}} = 3.9^\circ$ with no surface roughness and $\theta_{i,\text{eff}} = 15^\circ$ where $\sigma = 10^\circ$. Figure 13 also shows greater particle scatter, with an interquartile range in the $\sigma = 10^\circ$ case of 9.9° compared to 2.6° with no surface roughness.

The effect on total system deposition is shown in Figure 14, where the inclusion of surface roughness dramatically reduces the proportion of injected particles that stick. Note that the deposition fractions shown refer to the proportion of particles that enter each domain. The mass fraction of particles depositing throughout the whole domain fell from 92% with no surface roughness to a low of 33% where $\sigma = 5.0^\circ$. The best match to experimental data, shown by dotted lines in Figure 14, lies between $\sigma = 5.0^\circ$ and $\sigma = 7.5^\circ$. Whole system deposition at $\sigma = 5.0^\circ$ was 33% compared to 27% experimentally, whilst deposition in the first and second bends were 18% vs. 12% and 7.1% vs. 12% respectively. The overall drop in deposition is driven by the first bend, where the intermediately sized particles that adhere with a smooth wall appear to have sufficient normal velocity to overcome adhesion. This is shown by the distribution of particles throughout the domain in the authors' previous work [64]. The greater proportion of particles that adhere in the second bend supports the earlier conclusion that, without surface roughness, simply not enough particles were entering the region to generate realistic predictions of deposition. It should be noted that these simulations assume that the surface roughness is similar on all impacting surfaces. However, Wammack et al. [65] have shown that surface roughness develops non-monotonically with time as peaks are created with the valleys between them subsequently filled by further deposition. The influence of surface roughness, shown here, indicates that a future evolution and erosion model should include predictions of surface roughness evolution.

In summary, the introduction of surface roughness makes impacts more normal to the surface. This is particularly pronounced in the present system by the generally shallow actual impingement angles, θ_i , which average 3.9° . This led to an overall reduction in mass-fraction deposition, as a greater proportion of impacts are over the critical normal velocity. Results where $\sigma = 5.0^\circ$ more closely matched experimental data than the case without surface roughness. However, for quantitative validation of deposition predictions, further experimental data is required with a known roughness distribution.

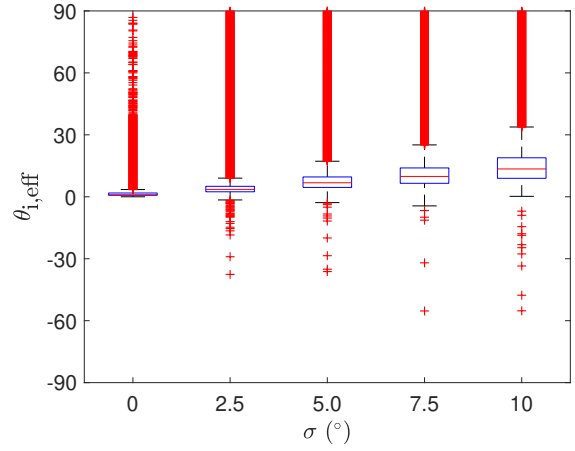


Fig. 13 Statistical distribution of effective impingement angles $\theta_{i,\text{eff}}$ from CFD.

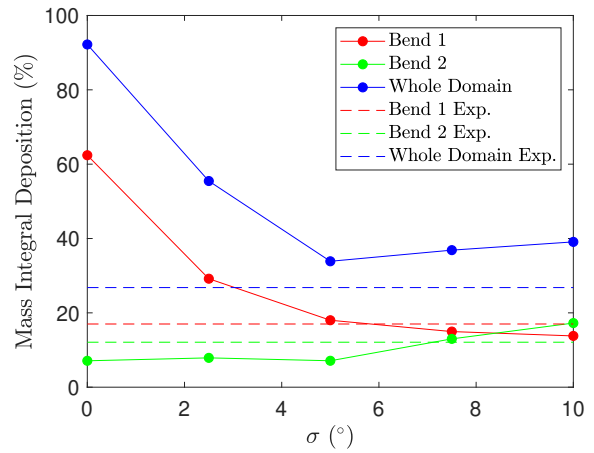


Fig. 14 Mass integral deposition for different regions of the domain. Note that deposition fractions refer to the mass of particulates that enter each region.

Non-Spherical Particles with Surface Roughness. Simulations were performed with surface roughness $\sigma = 5^\circ$, as in the previous subsection, with spheroidal particles of aspect ratio $AR = 1.9$. The initial orientation and angular velocity of the particles were determined from Equation 5 and the method described in the discrete phase methodology section. A probability distribution of particle initial orientation angles is shown in Figure 15. The trend is as expected from Equation 5 and Figure 11, where the particle is approximately four times as likely to impact with its major axis parallel to the surface ($\theta = 0^\circ$ or $\theta = -180^\circ$) as it is end-on ($\theta = -90^\circ$). The average angular velocity of the particles was 71% lower than the equivalent value for a sphere, predicted by Fluent from the model by Dennis et al. [66]. This agrees with the findings from the DNS studies discussed in the literature that non-spherical particles are likely to rotate more slowly, on average, than spheres.

Previous work by the authors [33] demonstrates the sensitivity of rebound trajectory to orientation angle, which is again shown by Figure 16. The outbound velocity normal to the surface is higher in many cases than the inbound normal velocity, reaching a maximum of $CoR_n = 2.5$ between $-20^\circ \leq \theta < 0^\circ$. Improbable as it may seem, this is the result of both surface roughness

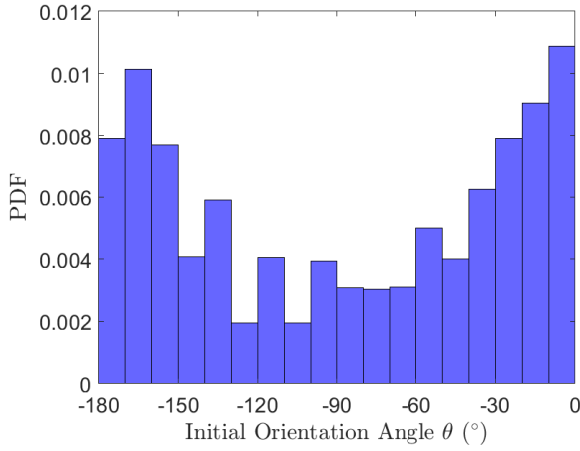


Fig. 15 Probability density function of prolate spheroid initial orientation angles. Angles $\theta = 0^\circ$ and $\theta = -180^\circ$ both denote the particle's major axis is parallel to the surface, whilst $\theta = -90^\circ$ is an end-on collision.

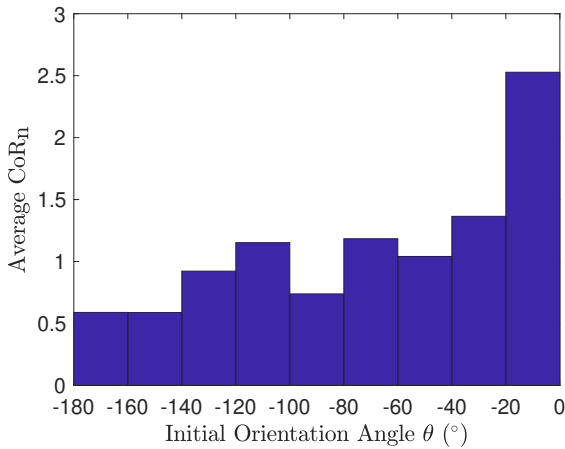


Fig. 16 Average normal coefficient of restitution for rebounding particles. Orientation angles $\theta = 0^\circ$ and $\theta = -180^\circ$ both denote the particle's major axis is parallel to the surface, whilst $\theta = -90^\circ$ is an end-on collision.

and non-sphericity. The previous subsection demonstrates that particles are more likely than not to collide with an inclined roughness structure, which ensures the transfer of momentum from the tangential component to the normal component. Hence, the CoR_n will be inflated at all orientation angles. The varying CoR_n with orientation angle is explained by the transfer between angular and linear forms of kinetic energy, or indeed momentum, as shown schematically in Figure 18. Where secondary collisions occur, angular velocity between the bounces is partially derived from friction with the surface, hence tangential momentum. Friction reduces tangential momentum, inducing an angular velocity about the particle centroid. Upon re-collision, this angular momentum (where the particle spins “into” the surface) is converted to normal momentum and hence increase the normal rebound velocity. This corresponds to the high CoR_n on the right hand side of Figure 16. Where only primary collisions occur, initial angular velocities provide momentum to increase

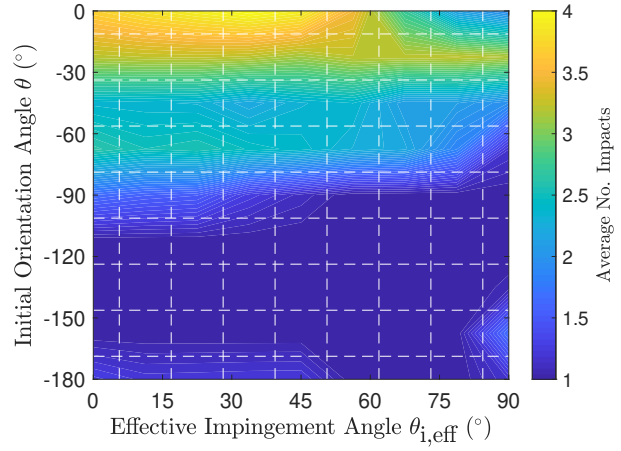


Fig. 17 Average number of impacts per collision event, for non-spherical particles.

the normal rebound velocity as shown by the right hand side of Figure 18. Total kinetic energy was conserved for all particles throughout multiple impacts, within the same collision event.

The average number of impacts experienced by a particle during a single collision event is shown by Figure 17. All recorded impacts from CFD were binned on a 10×10 grid of effective impingement and orientation angles. The frequency of secondary bounces is primarily a function of orientation angle, with impacts where the contact patch lags the centre of mass ($\theta > -90^\circ$, Figure 18) most likely to collide multiple times. This is because, as explained by the authors in [33], the rebound moment due to the normal force on the contact patch acts in the same direction as the moment due to friction, leading to the largest angular velocities. Particles with $-160^\circ \leq \theta < -110^\circ$ are likely to collide only a single time, due to their lower angular velocities at rebound but also the self-servo effect, discussed in the accompanying first part to this paper, which acts to increase the normal contact pressure. Higher impingement angles, hence more normal impacts, decrease the likelihood of secondary collisions by ensuring that the normal rebound velocity is sufficient for the particle to escape before it can “rotate into” the surface.

The predicted deposition distributions are shown in comparison to experimental deposition heights for the first and second bends in Figures 19 and 20 respectively. Experimental deposition is averaged over the same 6×6 grid used numerically to provide a like-for-like comparison. The resolution of the main deposition structure in CFD, Figure 19(b), is excellent when compared to the experimental deposition height, Figure 19(a). However, the overall deposit heights predicted are approximately two-thirds of those observed experimentally, peaking at $194 \mu\text{m}$ vs. $330 \mu\text{m}$. Despite the underprediction of integral deposition, the overall distribution of deposition is well predicted: both feature a broad peak at the top of the passage with a streak along the bottom edge. This difference is likely due to gravity. Both regions of deposition span the same proportion of the bend, at approximately two-thirds of the 90° bend. However, the peak of the numerical distribution is shifted 20° upstream compared to the experimental deposition.

The deposition distribution with the Magnus force disabled is shown in Figure 19(c). Without the Magnus force, the peak of deposition at the bottom of the passage is 30% greater at $253 \mu\text{m}$ vs. $194 \mu\text{m}$. Deposition at the top of the passage is also greater, peaking at $187 \mu\text{m}$. However, this is only an 11% increase over the

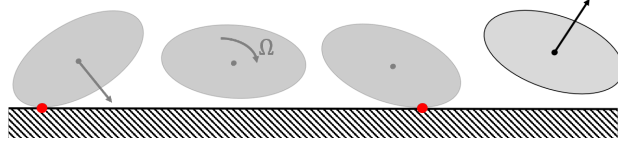
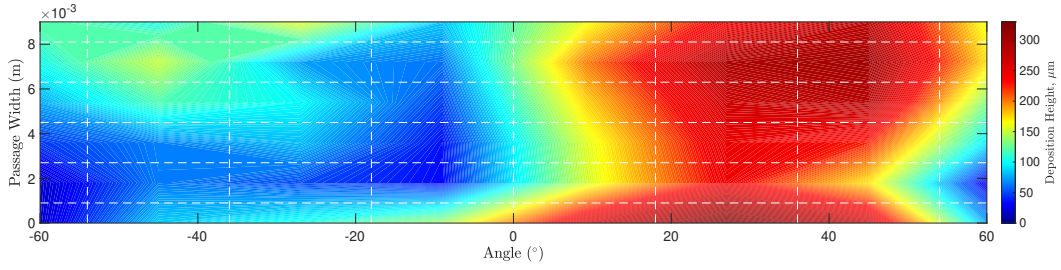
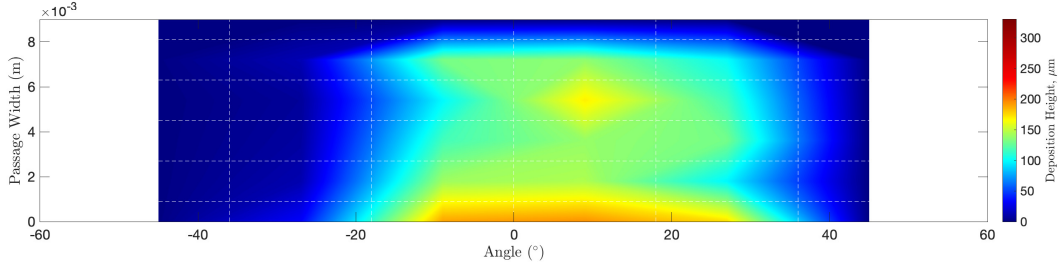


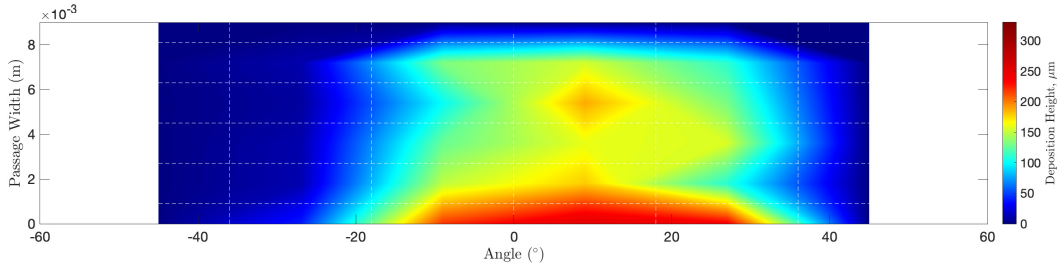
Fig. 18 Schematic showing a secondary collision. Note the transfer between linear and angular momentum.



(a) Experimental deposition distribution. Binned and smoothed to the same grid resolution as the numerical results. Raw scans in Figure 21.



(b) DEM/CRW predictions of deposit height with the Magnus force **enabled**.



(c) DEM/CRW predictions of deposit height with the Magnus force **disabled**.

Fig. 19 First bend outer wall: experimental deposition trends vs. numerical predictions for non-spherical particles (AR = 1.9) and a rough wall ($\sigma = 5^\circ$).

case with the Magnus force enabled. The same trend of increased deposition towards the bottom edge of the passage was seen in the authors' earlier work with spheres impacting a smooth wall [64].

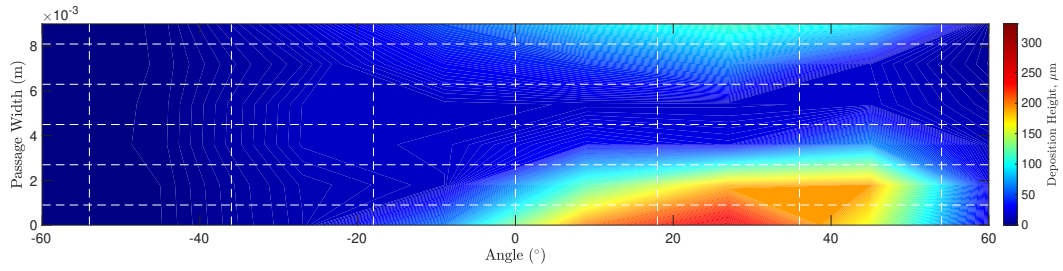
Deposition on the outer wall of the second bend is shown in Figure 20. As with the first bend, numerical predictions of the deposition structure (Figure 20(b)) are shifted upstream compared to the experimental results in Figure 20(a). In both cases, streaks of deposition are seen on the top and bottom edges of the passage, corresponding to the centres of the Dean vortices in Figure 5(b). In both, the peak at the bottom is higher than the top, likely due to gravity as in the first bend. The simulations predict greater deposition around the streaks than in experiments, spanning the centre of the passage. Quantitative agreement with experiments is similar to the first bend, with deposition peaking at $167 \mu\text{m}$ vs. $247 \mu\text{m}$.

Excluding the Magnus force, as seen in Figure 20(c), has a similar effect in the second bend to the first. Deposition is increased by approximately 30% and biased towards the bottom edge of the passage. Overall, this is a slight improvement in agreement with the experimental results. Further simulations with a Magnus lift

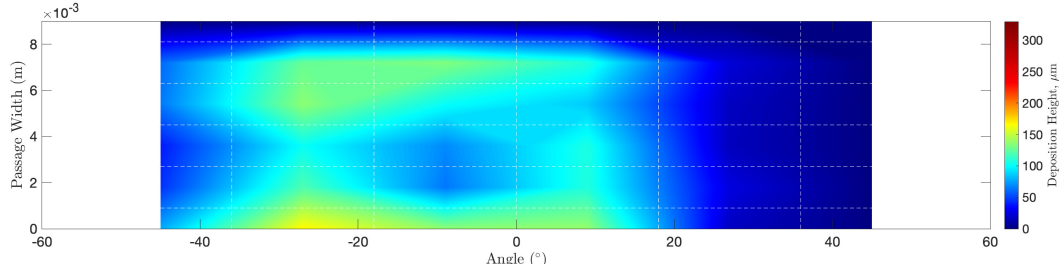
model that accounts for non-sphericity will be needed to fully assess the influence of collision-induced rotation on deposition distributions. However, it is clear that the effect of CIR and the Magnus force has a significant quantitative and qualitative effect on deposition.

The Alicona microscope scans of the bend surfaces are shown in Figure 21. The fine features of the experimental distribution are not captured with the 6×6 grid used to bin deposition numerically, however the grid resolution could be improved by injecting more particles as described in the methodology section. System properties like flow parameter reduction would likely be captured well by a low-resolution grid. High-resolution grids would likely be reserved for the detailed analysis of intricate geometries like double-walled cooling systems.

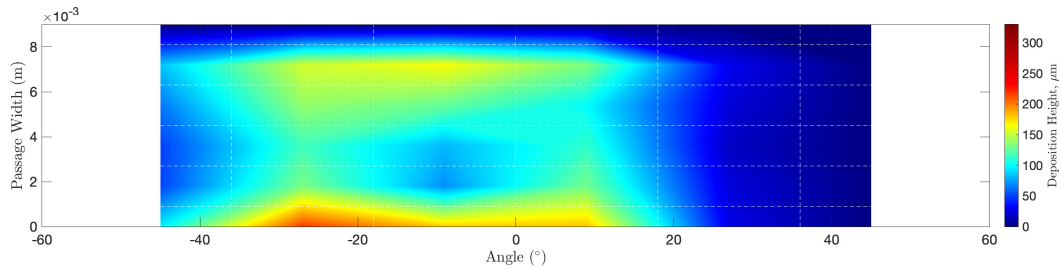
The quantitative predictions of deposition are a reasonable first-order estimation of passage blockage, which may be used in design. However, caution should be taken in drawing quantitative conclusions from such simulations. Fully validated packing or deposit evolution and erosion models are not implemented here. Notably



(a) Experimental deposition distribution, deposition height. Binned and smoothed to the same grid resolution as the numerical results. Raw scans in Figure 21.



(b) DEM/CRW predictions of deposit height with the Magnus force **enabled**.



(c) DEM/CRW predictions of deposit height with the Magnus force **disabled**.

Fig. 20 Second bend outer wall: experimental deposition trends vs. numerical predictions for non-spherical particles ($AR = 1.9$) and a rough wall ($\sigma = 5^\circ$).

however, the deposit heights predicted are significantly closer to experiment than those made for the same test case with spherical particles and a smooth wall [64] which over-predicted deposition height by a factor of three, leading to non-physical geometries (fully blocked passages). It is also notable that the experimental deposition height in Figure 19(a) is $> 10\%$ of the total passage height, which indicates that geometry and flowfield updating is required. In addition to correcting the flowfield disruption, a deposit evolution and erosion model would allow the inclusion of the following phenomena:

- erosion of existing deposition in the first bend by large incoming particulates;
- deposition on both clean walls and existing deposits with changing material properties and surface chemistry;
- insulation of the substrate by successive layers of deposition, increasing the wall temperature seen by incoming particulates;
- fluid shear causing deposit detachment.

Figure 22 shows how many times particles of different diameters are likely to bounce throughout the domain. Particles bounce 8 times on average, where those that rebound do so with an average normal coefficient of restitution of 1.17. The smallest particles, those less than a micron in diameter, adhere in 60% of first impacts with the modal number of impacts per particle increasing with diameter. The maximum number of impacts observed per particle was 43. The importance of an accurate bounce stick model is not

limited to local phenomena - inaccuracies in rebound predictions propagate downstream, affecting both the particle loading and the flowfield that the particle is subject to.

Figure 23 shows the integral mass fractions that deposit throughout the domain for different cases. These include simulations that use the Ohio State University and Critical Velocity deposition models, which will be discussed in more detail in the following subsection. Deposition for the DEM cases most closely matches the experimental results, at 14.0% compared to 26.8%, however still represents a significant underprediction. Exclusion of the Magnus force slightly increases integral deposition, to 14.6% for the whole domain. The authors' previous work on spherical particles showed that exclusion of the Magnus force decreased integral deposition by a factor of three [64]. The difference to the present results is likely due to the changes in CoR_n that results from non-sphericity and surface roughness, shown in Figure 16. Here the drivers are the length of time particles spend in the boundary layer vs. the bulk flow and the corresponding change in direction of the particle-fluid slip velocity. Notably non-spherical particles may also rotate in the opposite direction to spherical particles, as described by [33], which would reverse the direction of the lift force even where there is sufficient wall normal velocity for the particles to escape the bottom of the boundary layer. The underprediction of deposit heights in Figures 19 and 20 are of similar scale to the overall underprediction of integral mass fraction. This suggests that the distribution throughout the

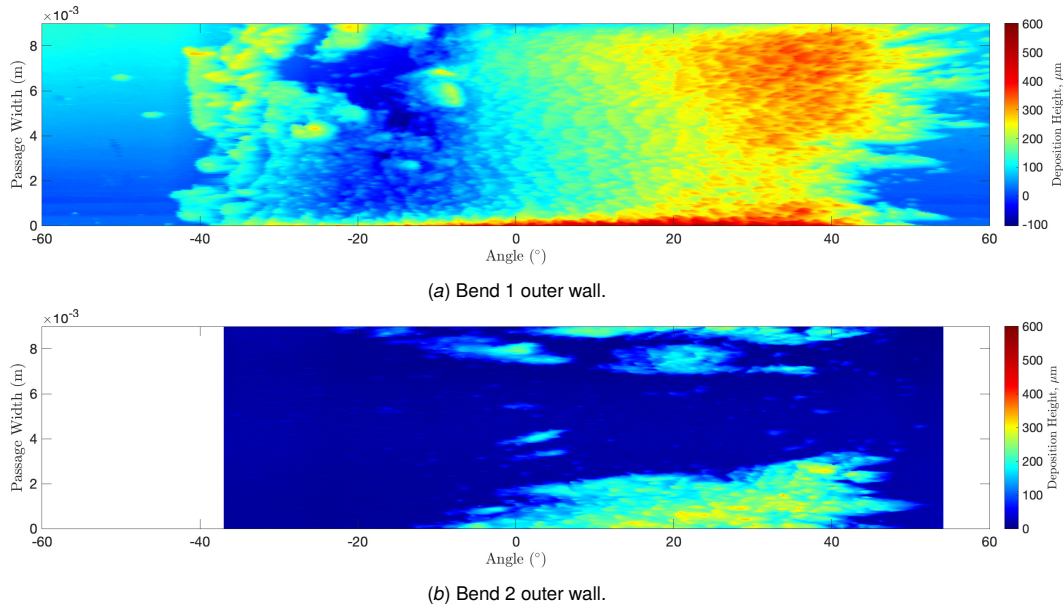


Fig. 21 Raw Alicona scans of the outer walls of both bends, which are binned and interpolated in Figures 19(a) and 20(a) to match the numerical approach.

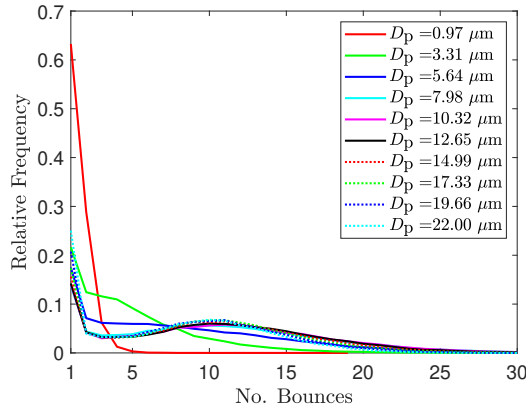


Fig. 22 The relative frequency of different numbers of wall collisions per particle throughout the domain. Note the x-axis is truncated for clarity, particles bounce up to 43 times each.

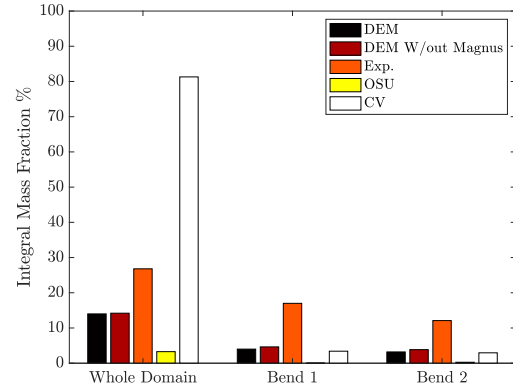


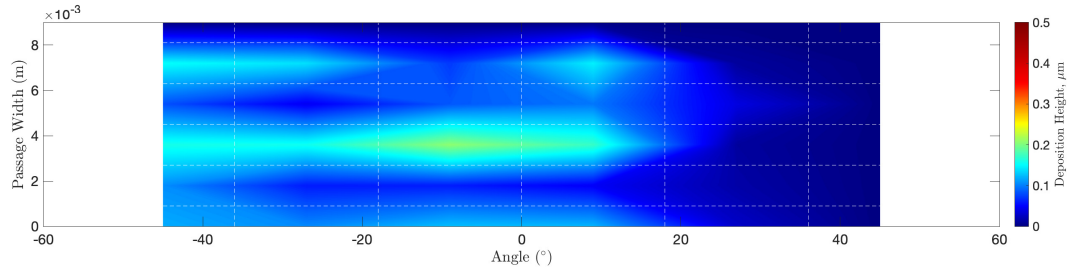
Fig. 23 Ratio between particle mass that deposits vs. enters different regions of the domain. Note that material parameters were not fitted for the OSU model.

passage is correct but the likelihood of stick for this material pair is underpredicted, perhaps owing to poorly understood material properties.

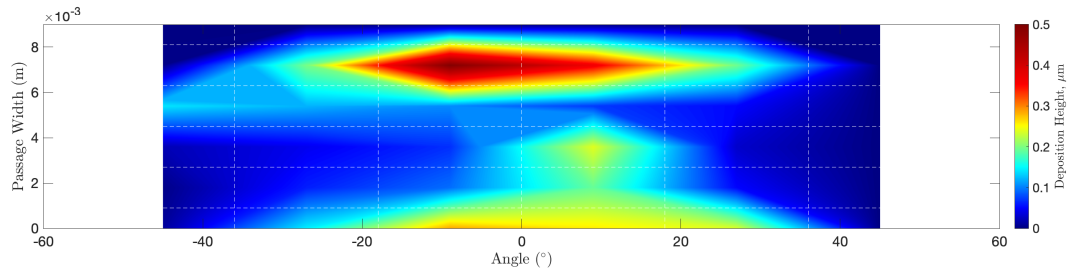
Bounce Stick Comparison. As a comparator, particle tracking simulations were also run with the OSU and CV bounce stick models. Material properties used for the OSU model were those proposed by Bons et al. [2]. Particle tracking simulations took approximately 8 hours with 1.3×10^6 particles for the OSU model, one third of that with DEM (including particle transport modelling). The CV model allowed for the fastest runtime at approximately four hours.

Results for the OSU model are shown in Figures 24(a) and 24(b) for the first and second bends respectively. The deposition heights predicted are approximately three orders of magnitude lower than the experimental results or DEM predictions. More deposition is observed in the upstream half of the bend, contradicting the

experimental distribution in Figure 19(a). However, peaks of deposition on either side of the passage are shown, as observed experimentally. This is particularly apparent in the second bend, which provides a good qualitative match to experimental results. In slight contrast to the experimental results for the second bend, greater deposition is predicted at the top of the passage vs. the bottom. Integral deposition fractions predicted by the OSU model were also orders of magnitude lower than for other models and experimental data (see Figure 23). However, it should be noted that no material properties were fitted to this dataset as was previous done by Bons et al., so it does not completely represent a like-for-like comparison between models. Comparing the DEM and OSU models, Gaskell et al. [3] found that the optimum value of surface free energy employed for each model varied by an order of magnitude. This is likely to be due to the semi-empirical nature by which the contact area is derived by Bons et al. Simulations that used the same material properties as the DEM model produced similar qualitative deposition distributions for both bends. The qualitative agreement between the OSU predictions of deposition

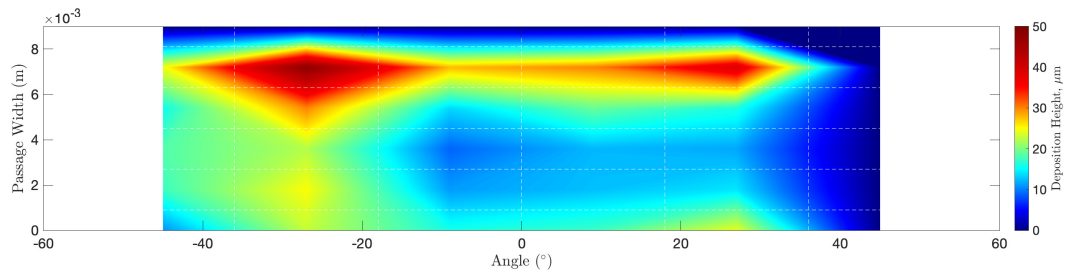


(a) First bend outer wall.

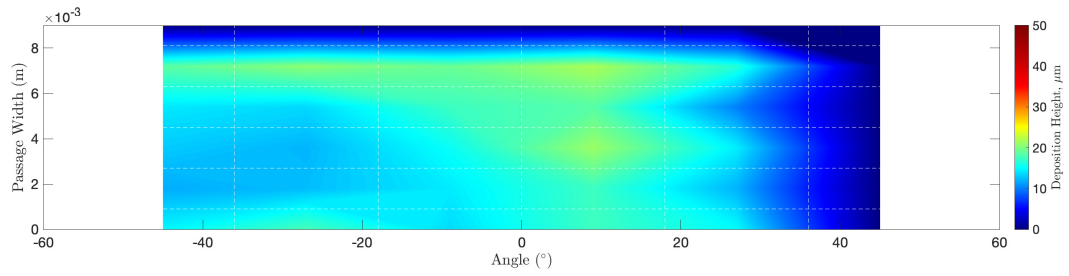


(b) Second bend outer wall.

Fig. 24 Predicted deposition heights on the outside wall of the first and second bends with the CRW and Ohio State University (OSU) models enabled.



(a) First bend outer wall.



(b) Second bend outer wall.

Fig. 25 Predicted deposition heights on the outside wall of the first and second bends with the CRW and Critical Velocity (CV) models enabled.

in the second bend and experimental data is encouraging, but what amounts to an all-stick condition may lead to less accurate predictions in inertia-dominated regimes.

The particle deposition trends produced by the Critical Velocity (CV) model are shown in Figure 25. The material parameters used were the same as for the DEM model based on the similarity of their CoR_n predictions for low velocity impacts [3]. Deposition in the first bend is skewed towards the top of the passage, however otherwise it is qualitatively similar to the OSU model with peak deposition on the upstream side of the bend and streaks matching the centre of the Dean vortices. Quantitative agreement is superior to the OSU model with peak deposition of 50 μm . However, this is still an order of magnitude less than the experimental observations. Reasonable qualitative agreement is shown between the CV and OSU predictions in the second bend: deposition is biased towards the top of the passage in the centre of the bend. Integral deposition is substantially higher than experimental values for the whole domain at 81.3% vs. 26.8%. Deposition in each bend was much lower at approximately 3%, implying that the majority of particles that deposit do so between the two bends. This was also observed for spherical particles using the DEM model in the authors' previous work [64]. Both energy-based models largely fail to capture the qualitative deposition trend from experimental data.

CONCLUSIONS

Particle tracking simulations and experimental data have been presented that are representative of deposition in a gas turbine secondary air system. Major flow features, Reynolds number, gas and metal temperatures, and particle size distributions are all similar to what might be expected of a typical HP blade cooling passage. This is the first application of the authors' DEM-based non-spherical bounce stick model to CFD and it represents the most complex flowfield to which the CRW turbulent transport model has been applied to date. Hence, a robust methodology is presented for the prediction of particulate deposition in gas turbine secondary air system components. All primary physical phenomena relevant to particle collisions, as determined by the authors' previous work, are incorporated. The ability to predict qualitative trends of deposition will allow improved predictions of performance degradation throughout fleet service life and the design of deposition-tolerant hardware. For example:

- prioritising surfaces for corrosion-resistant coatings;
- identifying regions of cooling passages where deposits may affect the rate of heat transfer;
- comparing the susceptibility of different geometries to particulate damage.

The results may also provide first-order approximations of quantitative deposition data, for example: deposit height; integral mass fraction deposited; and corresponding reductions of flow parameter in-use. The general trend of deposition heights was correct throughout the domain, but at approximately two-thirds of the experimental values. This suggests that the likelihood of stick for this material pair is underpredicted, perhaps owing to poorly understood material properties. To the authors' knowledge, these are the first comparisons between experimental and numerical deposition distributions for typical cooling flow regimes in the open literature. The conclusions of this work can be summarised as follows:

- Good qualitative agreement was seen between the deposition trends from the CRW/DEM approach and experimental data. With an average of approximately 8 bounces per particle, the accuracy of both models is crucial to predicting where deposition will occur. The approach demonstrates the ability to predict, to the first order: where particles impact; how they rebound; and what impacts are likely to result in adhesion.

- Deposition predicted by the DEM-based approach differed significantly from that of state of the art energy based models. Those produced by the DEM were qualitatively superior, however a more complete study that includes deposit evolution and packing factor is needed to quantitatively assess model accuracy.
- Surface roughness can be incorporated into CFD outside the collision model, by augmenting the particle angle of incidence. The method presented here accounts for the so-called "shadow-effect" with negligible computational cost compared to the collision model itself. As expected, this results in more normal impacts than with a smooth surface hence is shown to significantly reduce the integral mass fraction deposited. This appears to improve the relative deposition between different parts of the domain, however comparison with a component where the surface roughness is well profiled is needed to fully assess model accuracy. Significant scatter is also introduced into rebound predictions by surface roughness.
- A method to model the collisions of non-spherical particles in RANS CFD is shown, supported by the collision model derived in the accompanying first part of this work. Non-sphericity is shown to reduce the mass fraction deposited when compared to spheres and alter the qualitative distribution of deposition throughout the domain. The behaviour observed in FEA simulations of prolate spheroids was replicated by the CFD-DEM approach, notably the propensity of particles to impact the surface multiple times per collision event. This was shown to have a significant effect on rebound trajectories, with normal coefficients of restitution exceeding unity.
- Collision-induced rotation was shown have a modest but non-negligible effect on the qualitative deposition distribution. Quantitatively, its exclusion produced marginal increases in whole-system deposition. The results presented here validate the conclusions of Gaskell et al. [13], that particles in the boundary layer can be affected by CIR and should be included in bounce stick modelling. Differences between the effect of CIR for spherical and non-spherical particles warrants further investigation in future work.

Further work remains to capture additional drivers of deposition; most importantly the effects of deposit evolution and erosion. The DEM collision model provides a sound basis for further modelling, as it resolves all contact forces and surface pressures throughout the collision. Current tracking models are not capable of predicting the particle orientation angles required for accurate drag modelling and bounce stick predictions. Further work will extend the CRW model to track non-spherical particulates.

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Statement of Authorship for joint/multi-authored papers for PGR thesis

To appear at the end of each thesis chapter submitted as an article/paper

The statement shall describe the candidate's and co-authors' independent research contributions in the thesis publications. For each publication there should exist a complete statement that is to be filled out and signed by the candidate and supervisor (**only required where there isn't already a statement of contribution within the paper itself**).

Title of Paper	Modelling Particulate Deposition in Gas Turbines Part II: Prediction and Validation of Deposition Distributions
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Student Confirmation

Student Name:	Jack Graham Gaskell		
Contribution to the Paper	I developed the collision model used in the CFD simulations, adapted into a Fluent UDF with the help of Mr. Florian Villain, a fellow DPhil student at the OTI. I subsequently modified the collision model to consider surface roughness and predict the orientation and angular velocity of non-spherical particulates, which is a key contribution to knowledge of the work. The fluid solution I used to run the particle tracking simulations was produced by Dr. Nikul Vadgama, who had also developed the particle turbulent tracking model (CRW) used for the simulations. As first author, I also wrote the manuscript of the paper with limited sections from the CFD set up section adapted from Nikul's DPhil thesis, e.g. the mesh sensitivity study of the fluid solution.		
Signature		Date	23/8/2022

Supervisor Confirmation

By signing the Statement of Authorship, you are certifying that the candidate made a substantial contribution to the publication, and that the description described above is accurate.

Supervisor name and title: David Gillespie, Associate Professor		
Supervisor comments: The motivation for the research was prompted from the overall research aims of the group. Profs. Gillespie and McGilvray supervised the research, identified the overarching research strategy and liaised with Mr. Benjamin Littley, who provided industrial oversight from Rolls-Royce the industrial sponsor. Dr. N. Vadgama contributed to the development of the analytical particle transport models employed, and along with Mr. Simon Beal conducted the experimental work used in validation cases. Mr. F. Villain assisted in implementing the code in a commercial CFD solver.		
Signature		Date 23/8/2022

7 Summary, Conclusions and Further Work

The work reported in this thesis represents a significant advance in the modelling of particle surface interactions in the secondary air systems of gas turbine engines. Despite the prior development of physics based models it was not clear from these what physical phenomena needed to be included. For example, a physically unrealistic velocity dependence of the yield stress suggested by one approach implied that important aspects of the collision physics were not being captured. Similarly, the widely adopted assumption of particle sphericity has previously been made without an understanding of the sensitivity of rebound to that assumption. The current work demonstrates that the physics of colliding bodies are complex and highly coupled. Therefore, while it is recognised that some fitting of model parameters to experimental data may be unavoidable, there should be appropriate physical bases on which to do so. Fitting model parameters also drastically limits their use if appropriate experimental data is not available as is typical for novel material pairs, shapes or sizes. One clear improvement in the current work is the move away from energy-based models, which largely fail to capture the relevant collision physics and hence are unable to produce realistic predictions of deposition and subsequent particle trajectory.

7.1 Summary

The initial work conducted for this thesis sought to determine what inputs and outputs were required to accurately model rebound and deposition. This focussed on the conditions relevant to the secondary air system of gas turbines. Chapter 3 describes the sensitivity of particle trajectory to its rebound from the surface. The interaction between the solid and fluid phases near the wall demonstrate the importance of a model that accurately predict the coefficients of restitution and angular velocity in addition to the binary bounce stick criterion. The significance of the collision-induced rotation and the Magnus force on particle trajectory was identified and reported for the first time in the open literature.

Chapter 4 examined the sensitivity of particle rebound to shape. Particle shape can reduce CoR_n by up to 84 % compared to the spherical case, with transfers between linear and angular momentum that are not present for spheres. The propensity of a non-spherical particle to bounce multiple times

within a single collision event also leads to a highly discontinuous trend of rebound properties with orientation angle. Key differences in the collision physics between spherical and non-spherical particles were identified and used to develop the bounce stick model in Chapter 5.

A physics-based model was developed that incorporates all first order physical phenomena relevant to particle deposition in a gas turbine secondary air systems, presented in Chapter 5. Agreement between model predictions and experimental data is good with minimal reliance on empirical parametric fitting. It is able to predict the rebound of non-spherical particles deterministically and removes non-physical artificers of previous models. The time-stepping scheme allows all relevant collision physics to be coupled within the contact time and provides the flexibility to incorporate additional physical phenomena if needed, such as centrifugal forces as described in Appendix A.

A method of implementing the DEM model in CFD simulations has been developed, including the effects of surface roughness which are treated independently from the collision model itself. This is described in Chapter 6. A method of estimating the orientation and angular velocity of the non-spherical particles at impact was presented, based on the findings of existing DNS literature. The combination of the DEM collision model and the CRW turbulent transport model in CFD was found to provide excellent qualitative predictions of deposition distribution in comparison to experimental data when applied to a passage incorporating typical turbine blade cooling features. This will allow the susceptibility of different geometries to particle deposition to be established and spatial resolution and local areas of susceptibility to be established.

Reasonable quantitative predictions of deposition were also made with the approach, with predicted deposit heights approximately two thirds those of the experimental results. This was a significant improvement over the performance of existing energy-based collision models, which predicted deposition that was at least one order of magnitude less than observed experimentally, with poorer spatial resolution. Thus this may be used to generate first-order estimates of high-level characteristics such flow parameter reduction with engine life. Some inputs to the CFD simulations are still subject to significant uncertainty, particularly material properties, surface roughness and particle geometry. It is

likely that with improved input data the quantitative predictions would undergo substantial improvement.

7.2 Further Work

Ultimately, it is hoped that the simulation of particulate deposition in gas turbines will be a routine part of component design. Despite significant industrial need and interest in running such simulations, the computational overhead and modelling limitations of current numerical approaches are prohibitive to predict deposition height distributions locally in full engine components. The work presented in this thesis provides a substantial contribution towards detailed deposition modelling at the component level. Further work is required both in this area and also in complementary fields of turbulent transport modelling and deposit evolution and erosion modelling. The DEM model explicitly provides many formerly missing inputs to an erosion model, given its resolution of contact forces and pressures throughout the collision. Modelling techniques may always be refined and should be updated in response to further validation. Building on this thesis the steps below would further improve the fidelity of the predictive tools.

7.2.1 Detailed Study of Collision Induced Rotation employing both the DEM and CRW Models

The paper presented in Chapter 3 demonstrated that the Magnus force could not always be neglected in particle tracking, such is the influence of Collision-Induced Rotation (CIR). Subsequent research in Chapter 6 supports this conclusion, with qualitative and quantitative measures of deposition changing significantly when CIR was neglected. The methods used in Chapter 3 pre-date the development of the DEM model, hence exclude the effects of CoR_n , surface roughness and non-sphericity. They also exclude the CRW turbulent transport model, the development of which has also now reached maturity for use with RANS simulations. Thus replicating the work in Chapter 3, with these numerical tools and more realistic particle shapes would refine the characterisation of CIR in gas turbine components. Better understanding of residence time in the boundary layer, the effect of fluctuating slip velocities

in the presence of a more robust turbulent transport model will provide a more robust understanding of the effect of CIR on particle trajectory. This is important if a future lower order stochastic model is to be employed. The central conclusions are not likely to change.

7.2.2 Further Characterisation of Particle Shape Effects on Rebound and Deposition

Work presented in Chapter 4 finds three primary differences between spherical and non-spherical collision physics:

1. The existence of a rebound moment arm;
2. Different surface geometry at different particle orientations;
3. Particles may impact the surface multiple times per collision event, “secondary collisions”.

Based on this, prolate spheroids provide a shape that captures all primary differences between spherical and non-spherical particles, at a reasonable computational cost. All work published as part of this DPhil has examined particles with aspect ratio $AR = 1.9$, based on SEM imagery of collected atmospheric particulates. The computational efficiency of DEM compared to the original FEA in Chapter 4 provides the opportunity to model a range of particle aspect ratios. For example, the CFD simulations in Chapter 6 demonstrate that many secondary collisions may occur per particle. How this is likely to affect the rebound and deposition of particulates in real systems has not yet been established elsewhere in the open literature. Hence, a detailed comparison would provide an understanding of how different atmospheric contaminants are likely to deposit in-engine.

7.2.3 Quantitative Validation of Deposition Modelling

The experiments presented in the last chapter provide a quantitative comparison of numerical predictions with spatially resolved experimental data. However, due to the significant deposit volume, spanning approximately 10% of the passage height, the deposition cannot be fully decoupled from the flowfield. The effects of particle-on-particle deposition, in addition to heat transfer through the deposit, will also affect the accuracy of numerical predictions. Quantitative comparisons with CFD may be made where the mass of particles deposited experimentally is small, hence ensuring no significant change to the flowfield or heat transfer characteristics of the impacting surface. Detailed profiling of the surface roughness would also be beneficial to compare the effects of different surface

geometries experimentally, for comparison with numerical predictions. Such experiments would ideally be conducted with some form of particle tracking, for example Particle Shadow Velocimetry (PSV) or Particle Tracking Velocimetry (PTV). However, this would be extremely challenging if studying high-temperature deposition, which surely would be the aim for validity with in-engine conditions.

Such an experimental data set would also allow the effect of bounce stick model accuracy to be established. Whilst it is known from Chapter 6 that other bounce stick models in the open literature may fail to capture quantitative and qualitative deposition trends, it is not yet known quantitatively what the sensitivity of system deposition is to bounce stick predictions. It is proposed that further work would add noise to bounce stick predictions, for example $\pm 10\%$ of the predicted CoR_n . The distribution of deposition over surfaces of interest could be used to assess sensitivity, utilising the approach to spatial convergence proposed by Vadgama et al., 2020a. This will aid the development of future bounce stick models, by relating the predictions of single particle rebound like those in Chapter 5 to spatial distributions of deposition like those in Chapter 6.

7.2.4 Machine Learning of Bounce Stick Predictions

The collision of a non-rotating sphere and a smooth surface, for a given material pair, can be fully described by three parameters: total initial velocity, impingement angle and particle radius. Note that surface roughness is considered externally to the collision model itself, as described in Chapter 6. Based on the conclusions of Chapter 3, it can reasonably be assumed that the incoming angular velocity of the particle for this case is small. The three outputs of the collision model, in this case, are the normal and tangential coefficients of restitution, CoR_n and CoR_t , and the rebound angular velocity Ω . The full collision is therefore simply described - three inputs and three outputs. The collision physics, as described in Chapter 5, are highly coupled and complex but deterministic. It should therefore be possible to train a machine learning model to predict the three outputs from the three inputs, with less computational cost than running the DEM model directly. This is similar to the curve-fitting used by previous bounce stick models described in Chapter 2.5, however machine learning methods are proposed here to capture the complex collision physics shown in this thesis in

a computationally-efficient manner. Additionally considering non-spherical particles is conceptually identical, with additional input parameters.

This approach was trialled by the author in unpublished work, which demonstrated the potential of machine learning. The DEM model was used to pre-populate a large dataset of possible collisions, upon which a series of machine learning models were trained. Initially, the popular Python machine learning library Scikit-learn was used with a combination of regression models, for rebound predictions, and classification models, for prediction of the binary bounce stick criterion. The accuracy of the models for spheres was within the range that could be considered feasible for use in CFD: generally above 90 %. These have not been used further in the current work as there was no computationally-efficient way to incorporate the trained models into CFD: such are the limitations of memory management in ANSYS Fluent UDFs. Clearly this work should be generally applicable and approach has been shown to reduce the time taken to predict rebound by an order of magnitude compared to running the DEM model directly. Hence, for future generalised implementations of bounce stick machine learning from DEM should allow the simulation of systems with many more particles than resolving the collisions directly. The Machine Learning space could further be used along with a probabilistic mapping of collision conditions to generate a reduced order stick bounce model for preliminary design studies.

7.2.5 CRW Non-Spherical Particle Tracking

As described in Chapter 2.8, the transport of non-spherical particles in turbulence is highly complex. Most studies in the open literature directly resolve either the particle, fluid turbulence, or both to model their behaviour. For the purposes of particle transport, the work presented in Chapter 6 therefore assumes that the particles are spherical. The CRW model uses an RSM RANS solution to provide the relevant turbulent statistics for particle transport, and should be extended to allow particle orientation to be predicted throughout the domain, superseding the approximations made of particle orientation near the wall in Chapter 6. More importantly it would be useful to replicate the difference in wall-ward drift velocity observed experimentally and numerically between spherical and non-spherical particles, as described more fully in Chapter 2.8.

7.2.6 Implementation of a Robust Deposit Evolution and Erosion Model

Complementary to the focus of this thesis, work is required to develop a robust integrated strategy using the stick bounce model developed and existing CFD and erosion physics tools to simultaneously predict particle-on-particle deposition, erosion and deposit detachment due to fluid shear. The effects of surface roughness seen in Chapter 6 indicates that the evolution of surface roughness, as studied experimentally by Wammack et al., 2008, should also be included. The simulations should be conjugate, allowing for changed heat transfer through the surface as a result of the deposit. Advances in mesh-morphing have allowed some progress in this area, but reliable flow-field solution following the growth of large discrete deposits has to date been difficult to achieve. The ability to resolve all forces and contact pressures throughout the contact time would facilitate prediction of erosion, surface yielding and hence fracture of the impacting particle and surface, see Chapter 2.3.1.

7.2.7 Experimental and Numerical Investigation of Centrifugal Forces on Deposition and Rebound

Discrete Element Methods were used to develop the bounce stick model described in Chapter 5 partly to allow the inclusion of additional force-based phenomena. One such example was non-sphericity. Another is the effect of centrifugal forces, where particles impact a surface undergoing rotation. Note that the term centrifugal is used in place of centripetal as collision physics are most intuitively described from the particle frame of reference. A theoretical analysis of the effect of centrifugal forces on particle deposition and rebound is presented in Appendix A. In this initial consideration it is demonstrated that under certain conditions centrifugal forces may alter the pattern of deposition in a gas turbine component and hence should be included in bounce stick modelling. The DEM model has the ability to incorporate centrifugal forces, which are simply an additional term in the particle equations of motion. However, the implementation is necessarily case dependent as it will require the external definition of the impact location displacement from the axis of rotation and the global angular velocity. Hence, given the additional challenge of a current lack of experimental data for validation, it was not included in Chapter 6. Further work could examine this with a simple test case of a rotor-stator cavity. This would allow coupling to fluid effects that were neglected in Appendix A, which could be explored numerically in CFD and experimentally.

7.2.8 The Development of Low Order Probabilistic Models for Whole System Assessment

In this thesis the focus has been on changes experienced by a particle in response to individual surface collisions. For full engine modelling it is unfeasible to track sufficient particles through the air system to achieve an overall prediction of blockage in a secondary air system. With the ability to generate *à priori* arbitrary collisions in a multi-dimensional space, and to use the turbulent transport models to predict particle arrival at surfaces, it should be possible to generate probabilistic models of particle stick and transfer characteristics for typical air system components. This should allow preliminary design of air-systems to make them less vulnerable to blockage, with the explicit tools as described in this thesis then being employed to optimise the performance of the most vulnerable engine components.

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Appendix A Sensitivity of Particle Deposition to Centripetal Acceleration in Rotating Frames of Reference

The following paper has been submitted as a technical brief to the Journal of Turbomachinery. The models and simulations presented throughout this thesis and most existing literature assume that particles impact a stationary substrate. However, many components in the secondary air system of interest to deposition studies are rotating. Fluid flow in rotating frames of reference, like rotor-stator cavities, differ from the stationary frame of reference. However, how this affects particle motion is already considered by the Lagrangian particle tracking solver through drag. The work presented here is concerned with how a collision with a rotating surface differs from one that is stationary.

A series of low order models are developed which illustrate the differences between collisions in rotating and static frames of reference. As particle collision physics are most intuitively understood from the perspective of the particle, the rotating frame is referenced through the ‘fictitious’ centrifugal (CF) force. These CF forces are compared to other forces of interest, like the adhesive pull-off force and the average normal force that acts between the particle and surface during collisions.

The significance of CF forces was shown to differ between convex and concave rotating surfaces. In a gas turbine, examples of these include the hub of a rotor disk or its outer lip. The differences arise because the relevant force for comparison in the concave case is the average normal force, which is generally much greater than the adhesive pull-off force for comparison in the convex case. In both cases, the effect on rebound is small for large normal collision velocities. However, particles only adhere due to van der Waals forces at low collision velocities. Centrifugal forces were shown to affect the critical velocity at which particles stick. Monte Carlo-style simulations showed that particles were far more likely to deposit on the concave outer disk than the convex hub in an idealised rotor-stator cavity.

The results show that CF forces should be included in bounce stick modelling, where the collision occurs in a rotating frame of reference. The force-based nature of DEM model developed in Chapter 5 is well-suited for this, as CF forces are simply included with the addition of an extra term in the

particle equations of motion. The implementation in CFD would be case and geometry dependent, such is the need to specify the distance from the axis of rotation and angular velocity on a collision-by-collision basis.

DRAFT Particle Bounce Stick Behaviour in the Rotating Frame of Reference

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Particle deposition is a major damage mechanism for gas turbine components, especially in the secondary air system. Predicting the transport and deposition of ingested atmospheric contaminants is of great interest in component-level simulations during the design process. Bounce stick models predict deposition upon collision with a wall during Lagrangian particle tracking; they consider a range of physical phenomena, including van der Waals forces and plastic deformation. The effect of collisions in the rotating frame of reference, considering centrifugal forces, has thus far been neglected in the literature. That is despite the significant centrifugal loads experienced by many components of interest for deposition studies, for example turbine blades. The collision physics of the rotating frame are discussed here using low-order models and Monte Carlo-style simulations. The centrifugal (CF) forces experienced by the particle are shown to have a primary dependence on friction with the rotating surface. The CF forces were shown to have no dependence on the angular velocity or geometry of the rotating frame where a slip velocity exists between the particle and surface. No significant effect was found on the rebound velocities of particles experiencing “worst-case” CF forces. However, differences were observed in the sticking probability between concave and convex rotating surfaces, where the CF forces act in opposing directions to either push the particle into the surface or detach it. A force-based analogy of the popular Critical Velocity model was developed to study the phenomenon, considering CF forces. It was used in a Monte Carlo-style simulation of a rotor disk, finding that the variation of critical velocity due to CF forces was likely to bias deposition towards concave surfaces in the rotating frame. The collision physics of the rotating frame were found to be unintuitive, with complex implications for modelling deposition in gas turbine components. However, they were consequential in determining the distribution of deposition through the system, hence should be included in particle deposition simulations in CFD.

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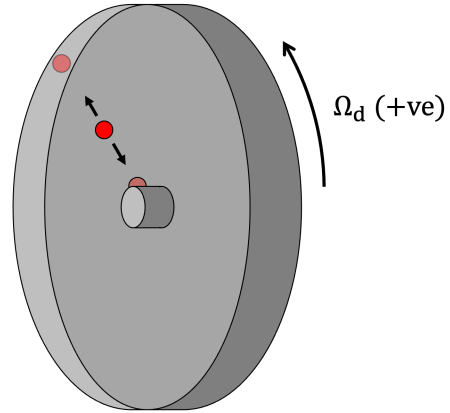


Fig. 1 Schematic of a particle impacting the concave and convex surfaces of a rotor disk.

Introduction

Gas turbines may ingest large quantities of atmospheric particulates throughout their fleet service life, which has been shown to accumulate in the secondary air and cooling systems [1]. This risks damage to hot-section components through the blockage of cooling passages, hot-spots caused by cold-side deposition, and corrosion. Temperatures in the secondary air system, at around 1000 °C [2–4], are sufficient to cause sticking but low enough to ensure multiple bounces per particle before adhesion. Previous work by the authors has shown that a particle may bounce eleven times on average in a secondary air system representative component, with each bounce affecting its subsequent trajectory [5, 6]. Modelling deposition in the secondary air system is therefore best suited to Lagrangian particle tracking simulations in CFD, as each trajectory is uniquely affected by the local flow and surface conditions.

The physics of particle rebound are complex and highly coupled. Primary physical phenomena to be considered are: plastic deformation, van der Waals adhesion, squeeze-film damping, friction and viscous damping. Secondary phenomena arise from surface roughness and particle non-sphericity, as described previously by the authors [7]. Van der Waals forces are the mechanism by which particles adhere, with other physical phenomena acting as energy loss or transfer mechanisms. This is the premise under which rebound is modelled by both the Critical Velocity (CV) [8] and Ohio State University (OSU) models [9]. A particle's kinetic energy at impact with the wall is converted to elastic potential energy as it compresses. If the energy that remains after losses like plastic deformation is not sufficient to overcome adhesion, the particle sticks. Otherwise, the particle rebounds with a kinetic energy that accounts for losses sustained during the collision. Exchange may occur between angular and linear forms of kinetic energy, meaning a non-spherical particle could - in theory - rebound with a greater linear velocity than when it first hit the surface [7].

Experimental deposition tests and simulations have largely been conducted on stationary components [10–12]. Vanishingly few studies consider that many gas turbine components are rotating at angular velocities of $O(10^3)$ rad s⁻¹. One such example is shown in Figure 1, where a particle impacts the concave and convex surfaces of a rotor disk. This will be the test case referenced throughout the following work. Dowd et al. [13] did simulate deposition in a rotating turbine blade passage, considering Coriolis forces. However, they only included its effect on particle transport, not the collision physics. To the authors' knowledge, no prior work has been conducted on the effect of the 'fictitious' centrifugal force on the likelihood of particle sticking, in this context. Note that

the centripetal force is the real force acting on a massive body undergoing circular motion, continually accelerating the body towards the centre of rotation. For example, when swinging a ball on a string, the tension on the string results from the centripetal force. The centrifugal force is the non-real force experienced by a body undergoing circular motion to correct for behaviour in the rotating frame. For example, when in a car turning left at speed one may feel as if they are being pushed to the right. As collision physics are most intuitively described from the perspective of the particle, all further references will be made to centrifugal force (CF).

This work specifically considers CF forces in the context of particle-surface interactions. When suspended in a fluid, the only forces that act on the particle are due to fluid effects like drag (assuming body forces like gravity, and magnetic and electrostatic effects are negligible). This is illustrated by considering a particle suspended in a rotating disk like that in Figure 1, in a total vacuum. Without contact with the wall, the angular velocity of the disk will have no effect on the particle. Commercial CFD solvers will solve the fluid phase considering system rotation, expressed on the particle through drag. Therefore, the only unresolved effects of the rotating frame will consider particle-surface interactions. Fluid effects are thereby neglected throughout this work, as they are already handled by the fluid-phase solver.

This paper examines the effect of centrifugal force on the deposition of spherical particles. The fundamental principles explained here may be later extended to account for non-sphericity. Low order methods and Monte Carlo simulations are used to determine whether deposition in a rotating frame differs from stationary components. How relevant effects may be included in bounce stick modelling is then discussed. What may seem like an innocuous question is shown to involve unintuitive physics with complex implications for the simulation of deposition in the rotating frame. The effect of centrifugal forces on rebound velocity are considered first, followed by the effect on sticking probability. The differing collision physics of impacts with concave and convex surfaces are also discussed.

Particle Kinematics in the Rotating Frame

A new sign convention is introduced to convert between the absolute and relative frames of reference, shown in Figure 2. A particle is shown impacting the concave surface of a disk like that in Figure 1, with the flat-plate analogy shown on the right hand side. Note that disk angular velocity Ω_d is positive in the counter-clockwise direction. The particle's total velocity is decomposed into normal and tangential components, with respect to the wall. The tangential velocity of the particle relative to the wall $V_{t,rel}$ is a function of its velocity in the absolute frame $V_{t,abs}$, the disk radius R_d and disk angular velocity Ω_d :

$$V_{t,rel} = V_{t,abs} - R_d \Omega_d. \quad (1)$$

It is assumed that the particle radius R is much less than R_d . The centrifugal force F_{cf} acting on the particle is therefore expressed as:

$$F_{cf} = \frac{m V_{t,abs}^2}{R_d} = \frac{m (V_{t,rel} + R_d \Omega_d)^2}{R_d}. \quad (2)$$

On the assumption that $|V_{t,abs}| < R_d \Omega_d$, the centrifugal force will be at a maximum where $V_{t,rel} = 0$. Therefore:

$$\max(F_{cf}) = m R_d \Omega_d^2. \quad (3)$$

The centrifugal force acting on the particle is therefore shown to be dependent entirely on the tangential behaviour of the particle, with respect to the surface. As will be shown later, this is true insofar

as the normal behaviour of the particle does not affect its tangential motion through friction, a second-order consideration. These principles are illustrated by considering the following thought experiments:

No Friction with the Wall. Where friction between the particle and surface is negligible, as shown in Figure 3, the collision in the rotating frame is indistinguishable from the flat plate analogy. Because there is no change in the absolute tangential velocity of the particle, there is no centrifugal force. In both cases, the particle will rebound along exactly the same path as its approach to the surface, with the same velocity in each case. Note that μ is the Coulomb coefficient of friction.

Infinite Friction with the Wall. Where friction between the particle and surface is infinite, as shown in Figure 4, upon collision with the disk the particle instantaneously accelerates to $V_{t,abs} = R_d \Omega_d$. It therefore achieves the maximum possible centrifugal force into the surface, $\max(F_{cf}) = m R_d \Omega_d^2$. This scenario assumes that the particle does not roll. The CF force it experiences may affect its rebound trajectory, assuming that the particle bounces, through greater losses due to adhesion or plastic deformation.

Clearly, in reality, the coefficient of friction lies between zero and infinity. However, zero and $m R_d \Omega_d^2$ bound the possible centrifugal forces experienced by the particle. As the centrifugal force is entirely dependent on a change in tangential absolute velocity, i.e. friction, the tangential impulse of the collision P_t must be considered:

$$P_t = m(V_{t3,abs} - V_{t0,abs}) = F_t t_{cont} = \mu F_{n,ave} t_{cont} \quad (4)$$

where the subscripts 0 and 3 denote before and following the collision, $F_{n,ave}$ is the average normal force acting on the particle during contact and t_{cont} is the contact time. The subscripts 0 and 3 are chosen to match the nomenclature of the authors' previous work, allowing for the effects of squeeze film damping [14]. Note that this case assumes that the particle slides throughout its contact with the wall, as is likely for an oblique collision. In a simplified example, assuming an elastic collision, the average normal force can be expressed through the component of impulse that is normal to the wall:

$$F_{n,ave} = \frac{2m(V_{n3} - V_{n0})}{t_{cont}} \approx \frac{2m V_{n0}}{t_{cont}}. \quad (5)$$

By substituting Equation 5 into Equation 4, the dependence on the contact time is removed. Assuming that the coefficient of friction μ and particle mass are fixed, the change in absolute tangential velocity of the particle is shown to have a primary dependence on the normal velocity of the particle:

$$P_t = 2m \mu V_{n0} \quad (6)$$

Therefore, at the first order, the centrifugal force experienced by the particle has no dependence on the disk radius R_d or angular velocity Ω_d . This is based on the assumption that the particle will slide throughout contact with the disk, the validity of which is discussed later. Maw et al. [15] describe the collision of an elastic sphere and half-space analytically. At low impingement angles θ_i (where the particle glances the surface), the particle will slide throughout contact. Maw et al. describes this process using two non-dimensional parameters:

$$\chi = \frac{7\kappa}{4} \quad (7)$$

$$\psi = \frac{\kappa}{\mu} \tan(\theta_i) \quad (8)$$

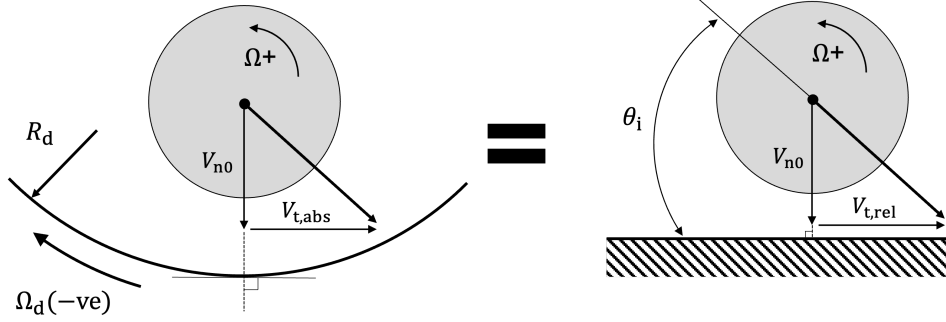


Fig. 2 Particle sign convention.

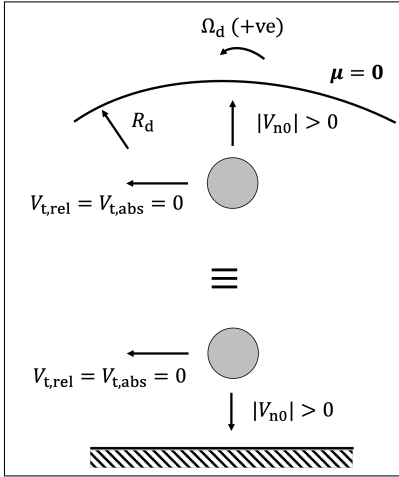


Fig. 3 Where friction with the surface is negligible, particle impacts in the rotating frame are physically identical to the stationary frame.

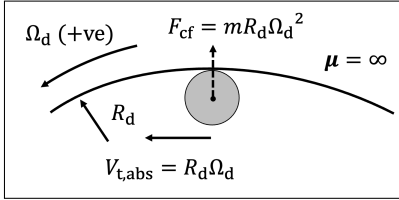


Fig. 4 Where friction with the surface is infinite, the particle instantaneously achieves the maximum CF force.

Where ψ is the non-dimensional impact angle and χ is a function of κ , the ratio of the particle's normal and tangential contact stiffnesses at impact. A model of κ for two dissimilar materials as proposed by Johnson [16] is used:

$$\kappa = \frac{\frac{1-\nu_1}{G_1} + \frac{1-\nu_2}{G_2}}{\frac{1-\nu_1/2}{G_1} + \frac{1-\nu_2/2}{G_2}} \quad (9)$$

Using the above parameters, Maw describes three patterns of behaviour for the collision of an elastic sphere and half-space:

- **Sliding regime:** $\psi > 4\chi - 1$
The contact patch is in gross slip throughout the collision.
- **Intermediate regime:** $1 < \psi < 4\chi - 1$
Contact starts with gross slip but reaches a no-slip condition during the collision (gross stick - note that this refers to the

slip velocity between particle and surface, not van der Waals adhesion). The point at which gross stick occurs gets earlier with increasing non-dimensional impingement angle (i.e. a more normal collision). After sticking, the contact patch reverts to gross slip before rebounding.

• **Sticking regime:** $\psi \leq 1$

The contact patch initially sticks to the surface, however after the midpoint of contact is passed and the particle starts to rebound gross slip is established before the particle rebounds.

By taking $\psi = 4\chi - 1$, the critical impingement angle at which no slip velocity exists between the particle and surface can be calculated as a function of solely material properties and the Coulomb coefficient of friction. From the authors' previous work [6], this is approximately mid-way between a normal and oblique collision (i.e. $\theta_i \approx 45^\circ$). The impingement angle θ_i will tend to a small value as Ω_d increases, as shown by Equation 1 and Figure 2. For example, an initial normal velocity $V_{n0} = 10 \text{ m s}^{-1}$ and initial absolute tangential velocity $V_{t0,abs} = 0$ corresponds to $\theta_i \approx 1^\circ$ where $\Omega_d = 10,000 \text{ RPM}$ and $R_d = 0.5 \text{ m}$. Therefore, where $V_{t,abs}$ is small compared to $R_d \Omega_d$, the centrifugal force is independent of the disk geometry and angular velocity. Not only is it independent of the disk angular velocity, it is also likely to be small compared to the maximum centrifugal force expressed in Equation 3. This is because low impingement angles (hence small normal collision velocities) imply a small tangential impulse, as discussed previously.

However, what if the particle impacts the surface with a small relative tangential velocity? Such a scenario is not unlikely if the particle bounces on a concave surface multiple times or is accelerated by the boundary layer near the disk surface. As discussed previously, $\max(F_{cf}) = m R_d \Omega_d^2$. This represents a "worst-case-scenario" for the effects of centrifugal force. By comparing the average normal force from Equation 5 with the maximum centrifugal force, the variable space over which centrifugal force may affect mean restitution can be determined. As the contact time is not known *a priori*, it is assumed to be equal to the elastic response time of the particle:

$$t_{\text{cont}} \approx t_e = 2R \left(\frac{\rho_p^2}{V_{n0} E_p^2} \right)^{1/5} \quad (10)$$

Substituting into $F_{n,ave}$ from Equation 5:

$$F_{n,ave} = \frac{2m(V_{n3} - V_{n0})}{t_{\text{cont}}} \approx \frac{2m V_{n0}}{t_{\text{cont}}} \approx \frac{4}{3} \pi R^2 \rho_p^{3/5} V_{n0}^{6/5} E_p^{2/5} \quad (11)$$

The ratio of average normal force and maximum centrifugal force is therefore:

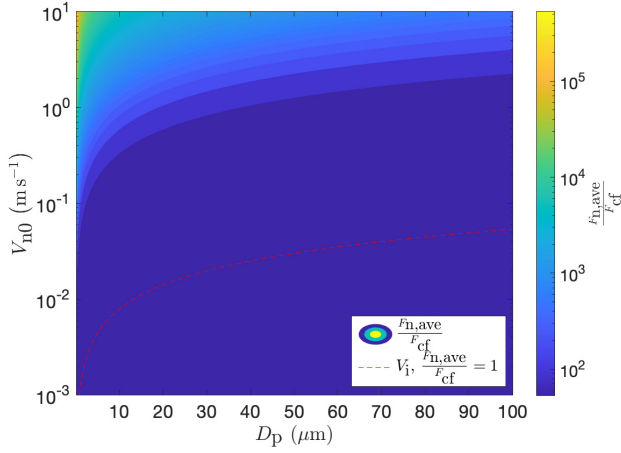


Fig. 5 The ratio of normal contact forces to centrifugal forces for a range of particle sizes and normal impact velocities. Case shown is for particles of Arizona Road Dust for $\Omega_d = 10,000$ RPM and $R_d = 0.5$ m.

$$\frac{F_{n,ave}}{F_{cf}} = \frac{V_{n0}^{6/5} E_p^{2/5}}{\rho_p^{2/5} \Omega_d^2 R_d R}. \quad (12)$$

By setting Equation 12 equal to one, the velocity at which centrifugal forces begin to dominate the collision physics V_i can be found:

$$V_i = \left[\frac{\rho_p^{2/5} \Omega_d^2 R_d R}{E_p^{2/5}} \right]^{5/6}. \quad (13)$$

These are both shown in Figure 5 for a range of particle radii and normal collision velocities. The particles used are Arizona Road Dust (ARD), a common test dust for gas turbine applications. The particles are assumed to be at ambient temperature with an elastic modulus $E_p = 96.5$ GPa and density $\rho_p = 2650$ kg m⁻³. Centrifugal forces are not significant for collision velocities greater than $O(0.1 \text{ m s}^{-1})$, which is a similar order of magnitude to the critical velocity at which large particles will stick due to van der Waals adhesion [9]. Therefore, while centrifugal forces are unlikely to affect particle rebound with large initial velocities, they may affect the critical velocity and rebound with low initial velocities. The effect of CF forces on critical velocity for adhesion will be explored later.

Detachment from Convex Surfaces

This work has, thus far, considered only particles impacting a concave surface. The effect of impacts on a convex surface, the hub in Figure 1, will now be considered. The relevant force for comparison with CF forces is then the adhesive pull-off force F_c , the force required to detach the particle from the surface at equilibrium [17]:

$$F_c = \frac{3}{2} \pi R \gamma \quad (14)$$

where $\gamma = 0.375 \text{ J m}^{-2}$ is the free energy between the particle and surface. Where a particle is already adhered to the surface, the condition $F_{cf} > F_c$ will ensure detachment. It follows that a particle impacting the surface with that condition will not adhere in the first place. Comparing the two forces:

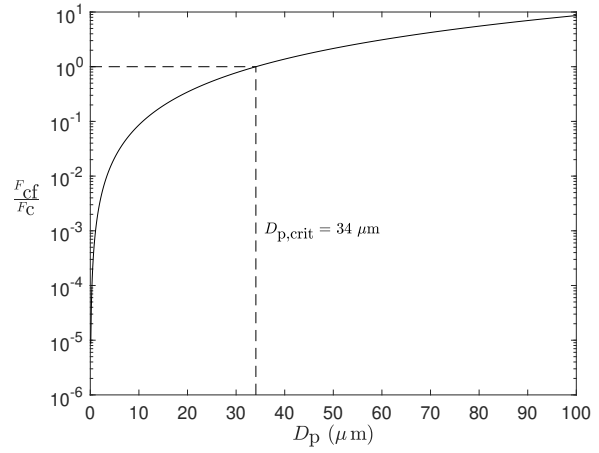


Fig. 6 Ratio of centrifugal force to adhesive pull-off force for ARD spheres vs. an SS316 substrate. Case shown is $\Omega_d = 10,000$ RPM and $R_d = 0.5$ m. Note that detachment will occur from a convex surface where $D_p \geq 34 \mu\text{m}$.

$$\frac{F_{cf}}{F_c} = \frac{8 \rho_p R^2 R_d \Omega_d^2}{9 \gamma} \quad (15)$$

the ratio F_{cf}/F_c can be used to estimate detachment. This is shown for ARD in Figure 6, assuming again that $\Omega_d = 10,000$ RPM and $R_d = 0.5$ m. The particle adhered to the surface will detach when its diameter is greater than $34 \mu\text{m}$. This is not significantly greater than the particles seen in the secondary air system of gas turbines, at approximately $10 \mu\text{m}$ [1]. This demonstrates that CF forces have a more significant role on convex surfaces than concave surfaces and are likely to cause detachment for large particles. Note that there is no dependence on particle velocity in Equation 15, in contrast to Equation 12.

Effect on Critical Velocity

It has been shown previously that centrifugal forces are unlikely to be significant when collision velocities are large. However, particles only adhere when collision velocities are small. Bons et al. [9] describe critical velocities for ARD $O(1 \text{ m s}^{-1})$. The binary nature of the bounce stick criterion means that a small change in critical velocity may cause substantial differences in the overall system deposition. The energy-based Critical Velocity (CV) model [8] provides experimentally validated [14] predictions of critical velocity and rebound velocity for the low speed normal impact of spheres. It compares the elastic potential energy stored in the particle, available to be converted to kinetic energy, to overcome the adhesive bond with the surface. However, centrifugal forces are not easily expressed in the energy domain. Therefore, an analogy to the CV model in the force domain is developed here using the average normal force throughout contact in Equation 11. This is compared with the adhesive pull-off force F_c :

$$\frac{F_{n,ave}}{F_c} = \frac{8 \rho_p^{3/5} R V_{n0}^{6/5} E_p^{2/5}}{9 \gamma} \quad (16)$$

assuming there is no relative velocity between the particle and surface. This expression is most intuitively described as the normal force between the particle and surface “pushing” it away, versus the adhesive force holding it back. It is proposed that where $F_{n,ave}/F_c > 1$, the particle will rebound. Where $F_{n,ave}/F_c \leq 1$, the

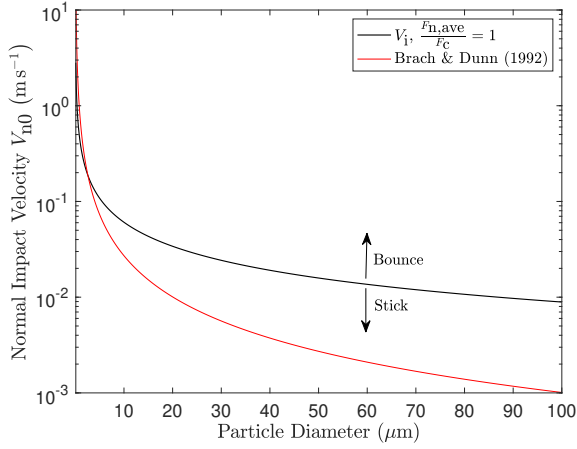


Fig. 7 Predictions of critical velocity from the force-based approach in Equation 17 vs. Brach and Dunn [8].

particle will adhere. Equation 16 can be rearranged to provide an approximation of the critical velocity in the absence of centrifugal forces:

$$V_i \approx \left[\frac{9\gamma}{8R\rho_p^{3/5}E_p^{2/5}} \right]^{5/6}. \quad (17)$$

The effects of centrifugal forces can also be included, opposing the effects of adhesion in the numerator of Equation 17:

$$\frac{F_{n,ave} \pm F_{cf}}{F_c} = \frac{(8\rho_p^{3/5}RV_i^{6/5}E_p^{2/5} \pm R^2\rho_pR_d\Omega_d^2)}{9\gamma}. \quad (18)$$

Equation 18 can also be rearranged to provide an approximation of the critical velocity in the presence of centrifugal forces:

$$V_i \approx \left[\frac{\frac{9\gamma}{8} \mp R^2\rho_pR_d\Omega_d^2}{R\rho_p^{3/5}E_p^{2/5}} \right]^{5/6}. \quad (19)$$

Figure 7 shows the critical velocity for ARD vs. SS316 stainless steel predicted by Equation 17, without centrifugal forces, to the predictions of the model presented by Brach and Dunn [8]. Particles that impact above the black critical velocity line will rebound, while those below will stick. Considering the log scale of the plots, the agreement is reasonable between the two approaches. The predictions from Equation 17 are always within one order of magnitude of those from Brach and Dunn, with material properties at ambient temperature from [5]. An empirical correction C aligns the two models:

$$C = 3.13 \times 10^{-4} \times R^{-0.60}.$$

Despite the reasonable match between the models, that the empirical correction is a function of the particle radius R implies that the force-based approach neglects some aspects of the collision physics. Therefore, it is not recommended that this approach is used in place of the critical velocity model for disparate cases without similar empirical corrections. The corrected model is shown against the CV model and predictions including CF forces in Figure 8. The critical velocity for concave and convex surfaces are shown by dashed and dotted lines respectively, where a lower line indicates a reduced propensity to adhere. Negligible differences are seen between the concave, convex and no CF force cases

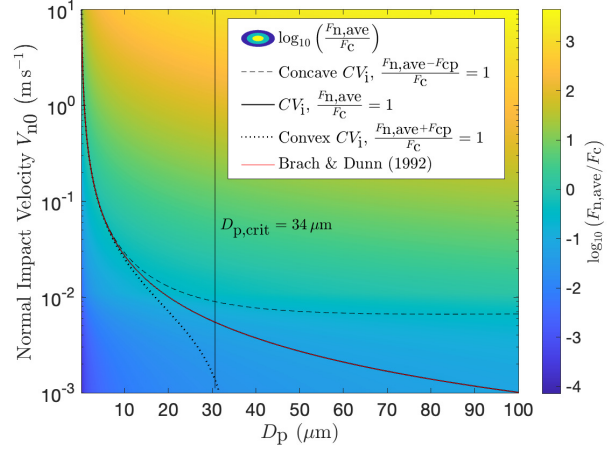


Fig. 8 Critical velocity for CF forces on the concave outer disk, convex hub and no CF forces. All critical velocities (Equations 17 & 19) are corrected by C to match the model from [8]. Contour shows the ratio of average normal contact forces to adhesive pull-off force.

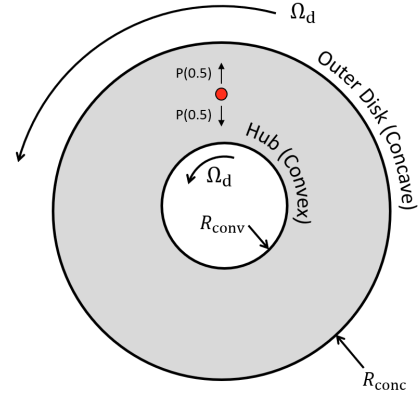


Fig. 9 Schematic of the rotor disk Monte Carlo simulation.

for particles below 10 μm in diameter. The critical velocity on the convex surface tends towards zero as the diameter approaches the critical value for detachment, as discussed previously. For the largest particles with diameter 100 μm, there is an order of magnitude error in the critical velocity when neglecting CF forces on the concave face. The contour in Figure 8 shows the ratio of average normal forces to the adhesive pull-off force. The ratio is shown to be at least 10 for all collision velocities greater than 0.1 m s⁻¹. This explains why CF forces are important for high velocity impacts on a rotating convex surface but not a concave surface: the relevant comparison is F_{cf} with $F_{n,ave}$, not F_{cf} with F_c . As the average normal force scales with the normal collision velocity, Equation 5, CF forces only become relevant at the smallest collision velocities in the concave case vs. across all collision velocities for the convex case.

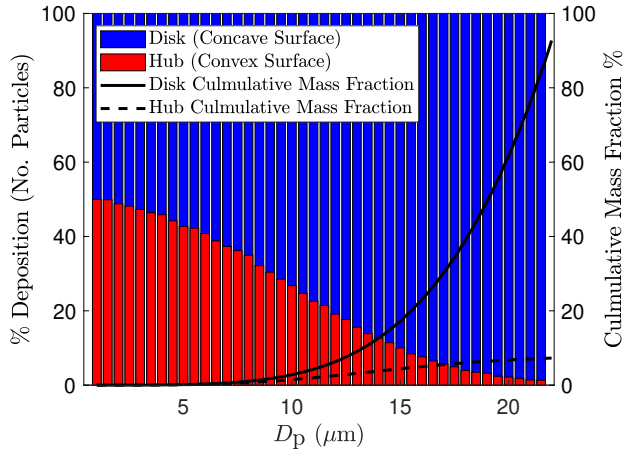


Fig. 10 Deposition on rotor concave (●) and convex (●) surfaces. Left y-axis and bars show deposition by particle number. Right y-axis and lines show cumulative mass fraction.

Particle Deposition Monte-Carlo Simulation

It has been shown that the rebound of particles with a large initial velocity is unlikely to be affected by CF forces, whether or not there exists a relative tangential velocity with the disk. Centrifugal forces have, however, been shown to affect the critical velocity at which the particle will adhere due to van der Waals forces. What effect this has on total system deposition for the rotor disk test case is now established, where $\Omega_d = 10,000 \text{ RPM}$. A Monte Carlo simulation is performed using the force-based critical velocity proposed in Equation 19. A schematic of the simulation is shown in Figure 9, where particles are injected mid way between the hub and disk rim with an equal probability of a velocity towards each surface. The particles have a random initial velocity and diameter from a uniform distribution: $0.010 \leq V_{n0} \leq 10 \text{ m s}^{-1}$ and $1.0 \leq D_p \leq 22 \mu\text{m}$. When a particle collides with either surface (the concave outer disk rim or convex hub), the impact velocity is compared with the critical velocity for that surface from Equation 19, corrected using C . If the velocity is below the critical value for that particle, it sticks and the process is repeated for a new particle. If the impact velocity is greater than the critical velocity then the particle rebounds with a stochastic normal coefficient of restitution (CoR_n):

$$\text{CoR}_n = \left| \frac{V_{n3}}{V_{n0}} \right| \quad (20)$$

from a normal distribution with a mean of 0.90 and a standard deviation of 0.20. The CoR_n is effectively the normalised wall-normal rebound velocity of the particle, with subscripts 0 and 3 chosen to match the nomenclature from [14]. This replicates the energy losses seen in real collisions, with the stochastic component replicating the spread of collision velocities seen in reality due to particle non-sphericity, surface roughness and local flow conditions. If it rebounds, the particle will collide with the opposing surface until it adheres to one of them. The particle is always assumed to collide with zero tangential relative velocity to the surface, as if accelerated by the boundary layer. This approximates a “worst case scenario” in terms of the effect of centrifugal forces. The radii of the concave outer disk rim and convex hub are both initially set to $R_{\text{conc}} = R_{\text{conv}} = 0.5 \text{ m}$. For the purposes of this thought experiment, this allows a fair comparison between centrifugal effects of a concave vs. convex surface without differing geometry. Therefore, any difference in the deposition between the two surfaces will be due to the effects

of CF forces, all else being equal between them. No fluid effects are considered.

The results are shown in Figure 10, in terms of the number of particles deposited per diameter and the cumulative mass fraction deposited on each surface. As may be expected from the critical velocities shown in Figure 8, the differing CF forces between the hub and outer disk make only a small difference for the smallest particles, those with a diameter less than $5 \mu\text{m}$. However, almost all of the largest $22 \mu\text{m}$ particles deposit on the outer disk rim rather than the hub. The disproportionate contribution of these large particles to the overall mass injected leads to over 90% of the particle mass to be deposited on the concave outer disk. This is despite the same distribution of particle sizes and velocities initially impacting each surface. As particles that rebound from one surface will re-impinge on the other, it is possible that the deposition bias is purely due to the propensity of particles to rebound from the hub and collide with the outer disk. That is, the concave disk rim itself has no greater likelihood of sticking than a non-rotating surface. However, reducing the hub radius R_{conv} to zero (hence reducing the centrifugal forces to zero, Equation 18), still results in approximately 80% of particle mass depositing on the outer disk rim. Therefore, CF forces are shown to increase the likelihood of deposition on concave surface as well as reduce the likelihood of deposition on convex surfaces. It also holds that this effect is significant for a realistic geometry, where the hub has a non-zero radius less than that of the outer disk.

All calculations thus far have assumed a rotor disk spinning at $\Omega_d = 10,000 \text{ RPM} = 1047 \text{ rad s}^{-1}$. Determining at what points in an engine cycle CF forces are relevant is of great use to determining their influence on engine performance. For example, how might the effect of CF forces vary between cruise and take-off conditions? Simulations like those in Figure 10 were performed for a range of disk speeds Ω_d , with and without corrections by C . The mass fractions deposited on the hub and outer disk for each are shown in Figure 11. A distinct cut-on effect is observed at $\Omega_d = 10^2 \text{ rad s}^{-1}$. At large disk speeds, all particles adhere to the outer disk with zero deposition on the hub. Likely HP turbine operating speeds are in the region most affected by CF forces, between 10^2 rad s^{-1} and 10^3 rad s^{-1} . This demonstrates the importance of including CF forces in bounce stick modelling for the relevant engine operating conditions.

Conclusions

Through a series of analytical calculations and the application of low-order models, corrected empirically, centrifugal forces are shown to affect particle bounce-stick behaviour in a specific range of circumstances:

- Where a particle slides throughout contact with a rotating surface (experiencing a significant tangential slip velocity), the CF forces experienced by the particle have no dependence on the disk angular velocity and radius. The only dependence is on friction, either through the Coulomb friction coefficient or normal contact forces.
- Where initial normal collision velocities are large, the worst-case CF forces are much less than the average normal force that acts between the particle and surface. Therefore, for impacts on a concave surface, rebound for large normal collision velocities is unlikely to be affected by CF forces.
- Particles adhered to a rotating convex surface are likely to detach due to CF forces, due to the dependence on adhesive pull-off force rather than compressive normal contact forces. For Arizona Road Dust, this is estimated to occur for particle

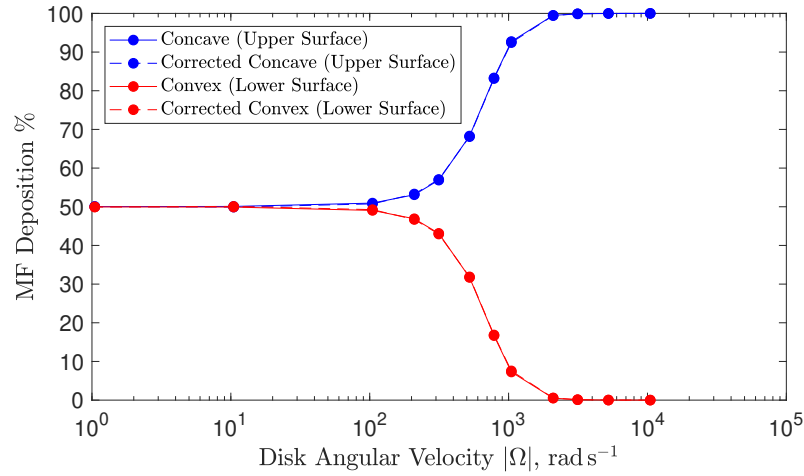


Fig. 11 Mass fraction deposited on the convex hub (●) and concave outer disk rim (●) for varying disk speeds Ω_d . Corrected values use a critical velocity (Equation 19) corrected by C . Disk and hub radii are equal $R_{\text{conc}} = R_{\text{conv}} = 0.5$ m. Note that 10,000 RPM ≈ 1047 rad s⁻¹.

diameters $D_p \geq 34 \mu\text{m}$ on a disk with radius $R_d = 0.5$ m and angular velocity $\Omega_d = 10,000$ RPM. It follows that particles greater than this size will not initially stick to the surface, when colliding with no initial relative tangential velocity. Distinctions must therefore be made between particle impacts on convex and concave rotating surfaces.

- Whilst impacts at large collision velocities are generally unaffected by CF forces, their effect on the critical velocity at which a particle will adhere due to van der Waals forces can affect overall system deposition. The critical velocity may vary by up to an order of magnitude, hence capturing many particles that would not otherwise have stuck. Concave and convex surfaces are equally affected. This leads to significant bias towards deposition on concave surfaces, where CF forces increase the critical velocity at which particles stick. For a rotor disk with a nominal radius of 0.5 m, this effect becomes significant at angular velocities greater than 10^2 rad s⁻¹.

These effects should be considered when modelling bounce stick behaviour in the rotating frame of reference. For example, when modelling deposition in turbine blade cooling passages or deposition on rotor disks. They are only relevant when the particle is in contact with a solid surface, as only fluid forces act on the particle when suspended in the flow. Further work should validate these predictions with experiments or CFD simulations with a validated bounce stick model.

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Statement of Authorship for joint/multi-authored papers for PGR thesis

To appear at the end of each thesis chapter submitted as an article/paper

The statement shall describe the candidate's and co-authors' independent research contributions in the thesis publications. For each publication there should exist a complete statement that is to be filled out and signed by the candidate and supervisor (**only required where there isn't already a statement of contribution within the paper itself**).

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Student Confirmation

Student Name:	Jack Graham Gaskell		
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Signature		Date	23/8/2022

Supervisor Confirmation

By signing the Statement of Authorship, you are certifying that the candidate made a substantial contribution to the publication, and that the description described above is accurate.

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Supervisor comments: The motivation for the research was prompted from the overall research aims of the group. Profs. Gillespie and McGilvray supervised the research, identified the overarching research strategy and liaised with Dr. John Irving, who provided industrial oversight from Rolls-Royce the industrial sponsor. Dr. Irving also supported the development of the model with insights from in-engine performance.			
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