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### FOUR-WAY COUPLING OF DENSE PARTICLES BEDS OF BLACK POWDER IN TURBULENT PIPE FLOWS

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#### ABSTRACT

*The modeling of particle deposition and transport in pipes is one of the most challenging problems in multiphase flow, because the underlying physics is multi-faceted and complex, including turbulence of the carrier phase, particle-turbulence interaction, particle-wall interactions, particle-particle interactions, two-way and four-way couplings, particle agglomeration, deposition and re-suspension. We will discuss these issues and present new routes for the modeling of particle collision stress. Practical examples like black powder deposition and transport in gas pipelines will be presented and discussed. The model employed is based on dense-particle formulation accounting for particle-turbulence interaction, particle-wall interactions, particle-particle interactions via a collision stress. The model solves the governing equations of the fluid phase using a continuum model and those of the particle phase using a Lagrangian model. Inter-particle interactions for dense particle flows with high volume fractions (from 1% to close packing ~60%) have been accounted for by mapping particle properties to an Eulerian grid and then mapping back computed stress tensors to particle positions. Turbulence within the continuum gas field was simulated using the V-LES (Very Large-Eddy Simulation) and full LES, which provides sufficient flow unsteadiness needed to disperse the particles and move the deposited bed.*

#### INTRODUCTION

Accurate prediction of particle dispersion in the atmosphere and in various engineering applications is very important in the assessment of human safety and in the analysis of risk. One of the engineering segments interested in acquiring accurate prediction tools for particle dispersion is the Oil and Gas industry, particularly in Black Powder deposition and transport in pressurized gas pipelines. Black powder[2] is toxic, with a

complex constitution, including radioactive elements. It consists of iron compounds such as magnetite and iron sulphide and includes sand and clay, salt, weld spatter and metallic iron. It is generated during gas production or in wet gas pipelines when hydrogen sulphide, carbon dioxide or oxygen is present in the gas, by bacterial corrosion of the steel, or from construction when lines are not cleaned adequately. It influences the flow performance of gas pipelines, impairs the function of valves and metering systems, and leads to severe accidents during transport.

In dense particle-bed systems, the flow behaves in a very subtle way, with very complex physical mechanisms near the wall, where the powder accumulates. A number of simplified analytical solutions to determine the conditions of particle-bed removal in pipes and channels have indeed been proposed, but with limited success due to the simplifications implied in these models. Today intensive research is devoted to understand the conditions for dense particle-bed formation and removal, in hydrocarbons and in many other related areas, like chemical engineering, but the difficulties encountered in measurements and flow visualization have hindered this progress. There are various incentives to explore the use of advanced prediction methods for this class of flows, featuring Lagrangian particle tracking including four-way coupling, instead of average Euler-Euler formulations, Large-Eddy Simulation (LES) instead of RANS, and transient rather than steady-state simulations.

In particle-laden pipelines, the particles tend to be transported through the pipeline by gas flow under specific conditions. The velocity required to move the particles could in some cases be estimated, made based on pipeline diameter, gas pressure, and particle size and density[1-3]. When black powder moves, it shatters and becomes very small in size, in the range of one micron or less, making it difficult to filter and possibly easier to move. Deposition of black powder will occur

if there are solids in the pipeline fluid and the velocity is not high enough to drag the particles along by viscous flow forces.

Sediment deposits can lead to blockage of the line, especially during pigging, while flowing powder can damage compressors, plug filters and damage user equipment. In some extreme cases, the piping could be half full of black powder, causing shutdown of the compressor and up to 60 tons of black powder could subsequently be removed from the piping.

This work aims at studying the mechanisms of turbulent dispersion, deposition and transport of solid particle in dense packed beds formed in 3D pipes. For the purpose, use has been made of the CMFD solver TransAT [4], a multiphase-flow dedicated computational fluid dynamics code. The physical model is introduced below. The mechanism of particle dispersion requires the turbulence in the carrier fluid phase to be modelled with a more sophisticated approach than RANS. In TransAT, we promote the use the V-LES and LES approaches, depending on the Reynolds number.

## THE PHYSICAL MODEL IN TRANSAT

### 2.1. Eulerian-Lagrangian dense particles model

The Eulerian-Lagrangian formulation for dense particle flows featuring non-negligible volume fractions ( $\alpha_p > 1\%$ ) in incompressible flow conditions is implemented in the CMFD code TransAT as follows (mass and momentum equations for the fluid phase and Lagrangian particle equation of motion):

$$\partial_t(\alpha\rho) + \partial_j(\alpha\rho\bar{u}_j) = 0 \quad (1)$$

$$\partial_t(\alpha\rho\bar{u}_i) + \partial_j(\alpha\rho\bar{u}_i\bar{u}_j) = \partial_j\alpha(\bar{\Pi}_{ij} - \tau_{ij}) + \bar{F}_b - \bar{F}_p \quad (2)$$

$$d_i(u_{p_i}) = -f_d \frac{9\mu}{2\rho_p d_p^2} (u_{p_i} - u_i[x_p(t)]) + g_i + F_{i, coll} \quad (3)$$

$$f_d = 1 + 0.15 \text{Re}_p^{2/3}$$

$$\text{Re}_p = \frac{\rho d_p \Delta U_{f-p}}{\mu}$$

where  $\alpha$  is the in-cell volume of fluid ( $\alpha + \alpha_p = 1$ ),  $u$  is the velocity of the carrier phase,  $u_p$  is the particle velocity,  $u[x_p]$  is the fluid velocity interpolated on to the particle position,  $\text{Re}_p$  is the particle Reynolds number,  $\Delta U_{f-p}$  is the relative velocity between the particle and fluid at the particle position,  $\Pi$  is the sum of viscous stress  $\sigma$  and pressure  $p$ ,  $\tau$  is the turbulent stress tensor (depending whether RANS, V-LES or LES is employed to deal with turbulence). Sources terms in (2) denote body forces,  $F_b$ , and the rate of momentum exchange per volume between the fluid and particle phases,  $F_p$ . Various drag correlations are available in the literature to account for higher volume fractions of particles; also the fluid viscosity can be modified based on the volume fraction of particles.

In (3),  $F_{coll}$  denotes the inter-particle stress. The momentum equation (2) presented here does not neglect viscous and

turbulent diffusion mechanisms in the fluid phase. The inter-phase drag model in (3) is set according to [5].

### 2.2. Four-way coupling modeling

The particle volume fraction is defined from the particle distribution function ( $\phi$ ) as

$$\alpha_p = \iiint \phi V_p dV_p d\rho_p du_p \quad (4)$$

The inter-phase momentum transfer function per volume in the fluid momentum equation (2) is

$$F_p = \iiint \phi V_p [A] dV_p d\rho_p du_p; \quad (5)$$

where  $A$  is the particle acceleration due to aerodynamic drag (1<sup>st</sup> term in the RHS of Eq. 3), i.e. excluding body forces and inter-particle stress forces (2<sup>nd</sup> and 3<sup>rd</sup> terms, respectively). The pressure gradient induced force perceived by the solids is not accounted for. The fluid-independent force  $F_{coll}$  is made dependent on the gradient of the inter-particle stress,  $\pi$ , using

$$F_{coll} = \nabla \pi / \rho_p \alpha_p \quad (6)$$

Collisions between particles are estimated by the isotropic part of the inter-particle stress (its off-diagonal elements are neglected.) In most of the models available in the literature,  $\pi$  is modelled as a continuum stress ([6]), viz.

$$\pi = \frac{P_s \alpha_p^{\beta(=2-5)}}{\max[\alpha_c - \alpha_p; \varepsilon(1 - \alpha_p)]} \quad (7)$$

In TransAT, the particle field is predicted in a Lagrangian way first, which enables defining the particle volume fraction (4) and inter-phase momentum transfer function (5), then high-order accurate interpolations are resorted to map the Eulerian field (to estimate  $\pi$ ), then back again to the Lagrangian system to determine  $F_{coll}$ . The constant,  $P_s$  has units of pressure, and  $\alpha_c$  is the particle volume fraction at close packing (typically specified to be 0.6), and constant  $\beta$  is set according to Auzerais *et al.* [7]. As the particle volume fraction approaches the close packing limit, the collision pressure increases non-linearly to a large value, thus preventing the particle volume fraction from going beyond the close packing limit ( $\alpha_c$ ).

The original expression by Harris and Crighton [6] was modified to remove the singularity at close pack by adding the expression in the denominator and to prevent the pressure from changing sign (Snider, 2001). The  $\varepsilon$  is a small number on the order of  $10^{-7}$ . The particle stress is unaffected by the modification except when the volume fraction approaches or exceeds close pack limit, which is somewhat arbitrary and depends on the size, shape, and ordering of the particles. This limit can actually be physically reached or slightly exceeded.

## THE NUMERICAL APPROACH IN TRANSAT

### 3.1. The CMFD Code TransAT

The CMFD code TransAT© developed at ASCOMP is a multi-physics, finite-volume code based on solving multi-fluid Navier-Stokes equations. The code uses structured multi-block meshes. OpenMP and MPI parallel based algorithm can be used. The grid arrangement is collocated and can thus handle more easily curvilinear skewed grids. The solver is pressure based (Projection Type), corrected using the Karki-Patankar technique for low-Mach number compressible flows. High-order time marching and convection schemes can be employed; up to third order Monotone schemes in space and 5<sup>th</sup> order Runge-Kutta time marching schemes.

Multiphase flows can be tackled using interface tracking for both laminar and turbulent flows (Level Set, VOF with interface reconstruction, and Phase Field), the phase averaged homogeneous mixture model (with Algebraic Slip), and the Lagrangian particle tracking (one-way, two-way, and four-way coupling, including with heat transfer).

To mesh complex geometries, use is made of the Immersed Surfaces Technology (IST) developed by ASCOMP GmbH and implemented in TransAT ([8]). The idea is inspired from Interface Tracking Method (ITM) for two-phase flows, in that the solid is described as the second ‘phase’ with its own thermo-mechanical properties. The technique has the major advantage to solve conjugate heat transfer problems. The solid is first immersed into a cubical grid covered by a Cartesian mesh. The solid is defined by its external boundaries using the solid level set function. Like in fluid-fluid flows, this function represents a distance to the wall surface; is zero at the surface, negative in the fluid and positive in the solid. The treatment of viscous shear at the solid surfaces is handled very much the same way as in all CFD codes.

To better resolve boundary layers, IST is complemented by the BMR (block mesh refinement) technique, where additional refined sub-blocks are automatically generated around solid surfaces; with dimensions made dependent on the Reynolds number (based on the boundary layer thickness) and desired  $y^+$  for wall treatment (low Re model, two-layer or wall functions). This combined method can save up to 75% grid cells in 3D, since it prevents clustering grids where unnecessary.

### 3.2. V-LES

The idea of V-LES ([9]) is to combine RANS and LES for specific flow portions, where the size of the most important scales can be identified (e.g. pipe diameter). Here the flow is decomposed into resolved and subscale part, the latter being dependent on the flow rather than the grid (in contrast to the sub-grid scale modelling in LES). Like the LES approach, larger scales than the characteristics flow scale are directly resolved, meaning actually no model is included. However, the sub-scale part is modelled, though with a more refined statistical turbulence model than the Smagorinsky one, because these sub-scales are not necessarily isotropic or independent of

the boundary conditions, as speculated in LES. Typically, two-equation or Reynolds Stress models can be applied.

The approach assumes that the Kolmogorov equilibrium spectrum applies to the sub-filter flow portion, which justifies the use of RANS models. The V-LES used in this study uses the  $k-\varepsilon$  model as a sub-filter model. The filter width is no longer related to the grid size, but is made related to a characteristics length-scale of the flow. Increasing the filter width beyond the largest length scales will lead to predictions similar to standard RANS models, whereas in the limit of a small filter-width (approaching the grid size) the model predictions should tend towards those of LES. If the filter width is smaller than the length scale of turbulence provided by the RANS model, then larger turbulent flow structures will be able to develop during the simulation, depending on the simulation parameters (e.g. grid, time stepping and order and accuracy of the schemes employed). The method as currently implemented in TransAT was proposed by Johansen *et al.* [10], who refer to it as Filtered-based unsteady RANS.

### 3.3. LES

Large Eddy Simulation is based on the concept of directly solving for all turbulent length scales that can be resolved (larger than the grid size) on a given mesh and modelling (statistically) the effect of the sub-grid scales. However, arbitrarily coarse grids cannot be used for LES due to the assumptions put forward while developing the sub-grid scale (SGS) models, namely: small-scale isotropy, independence of the SGS scales from the boundary and inflow conditions and diffusive, dissipative characteristics). The number of grid points needed for an accurate LES scales non-linearly with the Reynolds number. This makes LES currently too expensive for industrial turbulent flows. The LES or filtered Navier-Stokes equations are well known, and are not repeated here. The SGS model employed in this work is due to Nicoud and Ducros [11] which has shown better predictive performance than other models for wall flows.

## V-LES OF PARTICLES TRANSPORT IN A 3D PIPE

### 4.1. Problem setup and modeling

Particle transport from bed

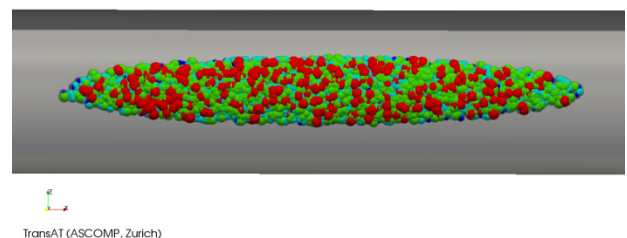


Figure 1. Initialization of the particle bed; the particles are colored by their size: top side view of the bed.

The objective of this section is to estimate/predict the critical velocity of dust transport in gas pipelines based on calculations. From the modelling point of view, the goal is to come up with the correct modelling requirements which allow the estimation of the critical velocity. The critical velocity is defined as the gas velocity needed to transport 10% of the initially injected dust mass from the starting point to the filter separator. Gas composition, gas temperature and dust characteristics are kept constant. Simulations were performed for one experimental condition ([12]) of gas flow at system pressure of 10 bars and gas temperature of 20°C. Further details of the experiments are not discussed in this paper; only limited amount of data was made available to the authors. The simulations involved changing the gas superficial velocity. The other flow parameters considered are:

- Length of dust layer: 1 m
- Dust layer thickness: 1–2 mm
- Dust material density: 2650 kg/m<sup>3</sup>
- Dust size: 200 – 400 μm
- Initial dust mass: 20 g

The gas flow field was solved using a V-LES approach with unsteady inflow conditions, as introduced previously. The dust mass was modelling using Lagrangian particle tracking (1-3). The 4-way mass and momentum coupling between the dust and gas phases was accounted for based on the model of Snider [13,14]. In this model the inter-particle collision is not directly simulated, instead a collision–pressure stress is introduced that indirectly takes into account the close–packing of particles.

## 4.2. Discussion of the results

The dust bed was initialized as a smooth bump as specified (see Fig. 1). Particles of 4 different diameters were used to represent the particle size distribution: 225, 275, 325, 375 μm. Inflow gas velocities of 2, 3, 5, 10 m/s were used. Each simulation was run for 10'000 iterations, with different time steps to adhere to the CFL criterion, for real times of 25, 16, 9, and 4.2 seconds, respectively. For the higher velocity cases, viz. 5 and 10 m/s significant fractions of particles had already left the simulation domain in the simulated time. For the lower velocities a quasi-steady rate of particles leaving the simulation domain.

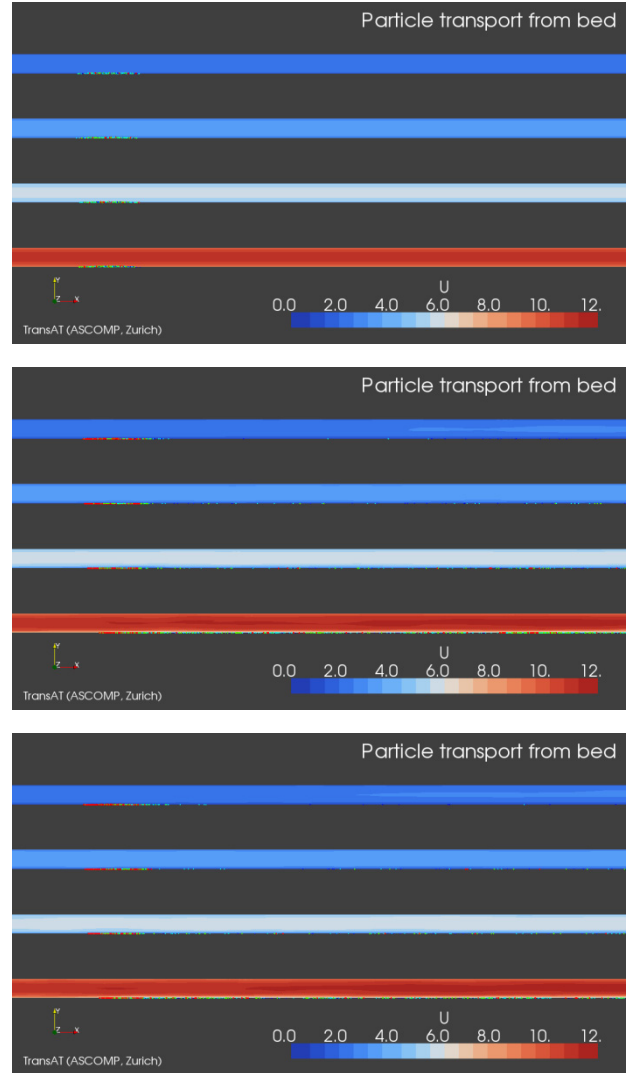


Figure 2. Snapshots of the simulations at 4 different times for 3 different gas velocities; velocities in m/s

Figure 2 shows that particles are moved by the flow along the pipe. However, all the particle transport takes place along the wall of the pipe. Very little particle entrainment into the core flow is observed. Particles are transported further in the pipe with increasing gas velocity, still without re-entrainment.

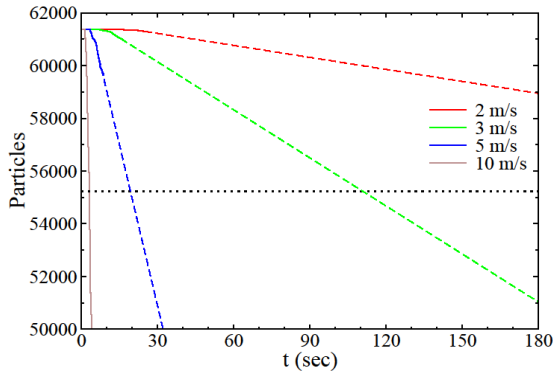


Figure 3. Number of particles remaining in the domain

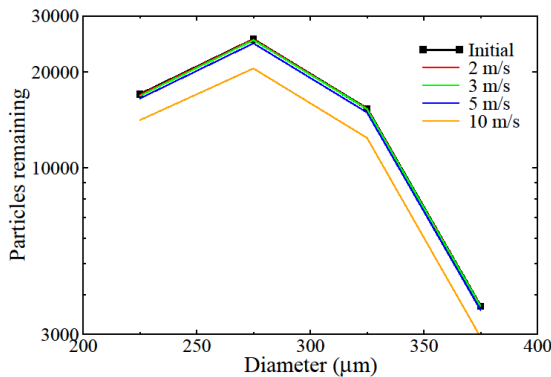


Figure 4. Number of particles still remaining in the pipe at the end of the simulation

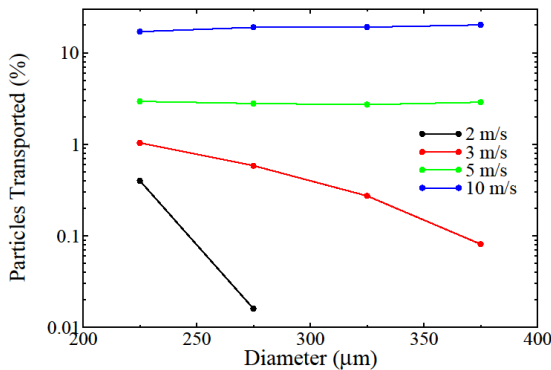


Figure 5. Percentage of particles transported out based on the initial number of particles

Changing the V-LES model parameterization has not helped lift-up of the particles. The critical velocity of transport was estimated by extrapolating the rate of change of particles in the domain to 3 min, from the simulated time. This is presented in Fig. 3. It can be inferred from this graph that the critical velocity (defined as 10% particle transport in 3 min) is around 3 m/s or slightly lower.

In the graph, the dashed part of the lines is linearly extrapolated results from the simulation. It was assumed that the simulations were run long enough to reach a quasi-steady state of particle removal. Even with the particles not being lifted-up in the core flow, the predicted value of the critical velocity matches exactly the measured value. The size

distribution of particles at the exit of pipe for critical transport conditions is shown in Figs. 4 and 5. All the values are taken at the end of the simulation period, which is different for different inlet velocities.

Figure 5 in particular shows that at low velocities, a larger fraction of smaller particles are transported, whereas at higher velocities an equal fraction of all particle sizes is transported. A larger difference in relative transport would be evident if a larger range in particle sizes is considered. In the simulated cases, the 4 diameter values considered are not that different (225–375 $\mu\text{m}$ ). The particles size distribution was assumed to be Gaussian with a mean diameter of 300 $\mu\text{m}$  and a standard deviation of 50 $\mu\text{m}$ . The particles were randomly initialised in the initial particle bed volume as shown in Fig. 1. In summary, it seems that the rate of particle-stripping from the bed is actually well simulated together with the critical transport velocity, even if the particle cloud has not lifted up.

### LES OF PARTICLES TRANSPORT IN A CHANNEL

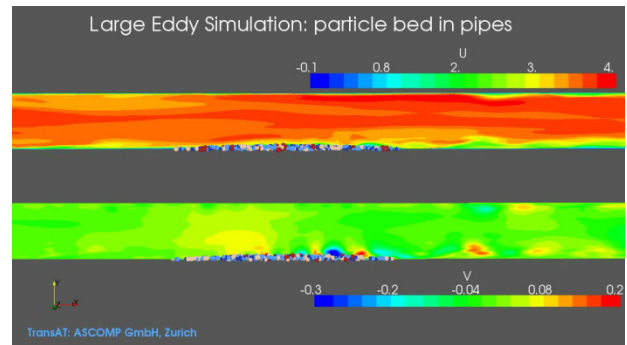


Figure 6. Particle transport in channel (4-way coupling); velocities in m/s

We present here first attempts to resolve the flow using LES of the gas flow in the pipe, instead of V-LES. Pursuing the flow analysis in this direction is motivated by the perception that small-scale turbulence (modelled by V-LES) may be responsible for lifting-up the particle cloud. The Lagrangian particle module is kept the same as explained previously; 4-way coupling. The SGS model for fluid flow turbulence was treated with the Nicoud & Ducros [11] model. No SGS model has been used for particle motion equation. A channel flow was simulated with initial fluid flow conditions exactly as in Narayanan *et al.* [15]. Periodic boundary conditions were set. The initialization of the particle bed was done as in the V-LES case, based on a log-normal distribution of the particles.

Snapshots of the flow obtained with the model are presented in Fig. 6 below, depicting particle concentration in the bed (coloured by their size) and the flow developed through the interaction with the carrier phase. Turbulence structures generated subsequent to the interaction are better highlighted with the vertical velocity contours (lower panel). Again, it seems that even with full LES, the particle re-entrainment in the

core flow is not captured, even if the negative vertical velocity magnitude reaches about 5 to 8% the maximum streamwise velocity, which is rather high compared to single-phase LES of channel flow. This means that other physical mechanisms are still missing to build up a complete model.

## CONCLUSIONS

The paper presents a simulation campaign of a turbulent gas pipe-flow laden with solid particles of different size, under different system pressure levels. The rate of particle-stripping from the bed is well simulated, and the prediction of the critical transport velocity is in line with the experiment, even if the speculated re-suspension of solid particles is not observed, either with VLES or LES. The reasons for the inability of capturing particle entrainment could be the following:

- The particle bed is too thin ( $\approx 2$  mm) implying 4–5 dust particle layers for the given maximum particle size of  $400\mu$ , requiring very high grid resolution.
- The particles are relatively large and gravity has a strong impact on their motion bringing them to the pipe floor quickly.
- Also, in the case of particles being ejected from the bed, since they are already very close to the wall ( $\frac{1}{4}$  mm), they do not develop any vertical velocity due to gravitational acceleration. This means that wall collisions might not contribute to resuspension.
- For particles that are much heavier than the fluid the Saffman lift force is known to be negligible. This was also tested as part of the model development effort.
- Accounting for wall roughness or dust non-sphericity might be important to obtain sustained particle suspension ([16]).
- Particle rotation is not accounted for in the simulations. If the particle rotation is high, then it can affect the wall rebound characteristics and also produce the additional Magnus lift force.

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