Thesis for The Degree of Licentiate of Engineering

Modeling and Analysis of Long-Term Particle Deposition on a Cylinder

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Particle-laden flow around a cylinder, with some particles deposited on the cylinder surface.

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To my family

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Abstract

Long-term particle deposition studies are challenging to conduct due to both their experimental and computational difficulties. In terms of computational challenges, the main difficulty is the extreme computational cost of accurate particle deposition simulations, where simulating the carrier fluid represents a large fraction of the total computational cost. This project investigates the potential of using the recurrence computational fluid dynamics (rCFD) method for time-extrapolating the carrier flow fields, eliminating a large fraction of the computational cost of particle deposition simulations.

Firstly, we investigate the feasibility and computational cost of using rCFD for performing a particle deposition study on a benchmark system of flow around a cylinder. In this study we show that deposition rates can be accurately obtained with rCFD at a fraction of the computational cost of conventional computational fluid dynamics (CFD). Special effort is focused on the cylinder back-side deposition rates, a benchmark case that is particularly challenging due to the turbulent wake interactions.

Secondly, we investigate the time-dependence of particle deposition rates on the back of the cylinder using direct numerical simulation (DNS) simulations. The results of this study indicate that particle deposition rates are highly time-dependent, with observed short-term impact rate fluctuations of up to a factor 27 for flow at $\mathrm{Re} = 6600$. To the best of our knowledge, this effect has not been observed before. This study emphasizes the importance of choosing an appropriate rCFD database, while at the same time highlighting the challenges in constructing such a database.

The aim of this project is to reduce the computational cost of performing particle deposition studies. Such a reduction in cost would be useful in academia and industry alike. Examples of applications include sensor soiling in the car industry, icing on aircraft and ash build-up in boilers.

Keywords

recurrence CFD, data-assisted simulation, particle deposition

List of Publications

Appended publications

This thesis is based on the following publications:

[**Paper I**] **J. Hansson**, T. Lichtenegger, S. Pirker, S. Sasic, H.Ström, *Recurrence CFD for efficient predictions of long-term particle deposition on a cylinder*
Submitted to a scientific journal.

[**Paper II**] **J. Hansson**, S. Sasic, H. Ström, *Low-frequency wake modulation governs particle back-side deposition on cylinders*
To be submitted to a scientific journal.

List of Conference contributions

Parts of this work have been presented at the following scientific conferences:

- The Swedish Mechanics Days (SMD). Gothenburg, Sweden. June 2024.
- International Conference on Numerical Methods in Multiphase Flows (ICNMMF). Reykjavik, Iceland. June 2024.
- International Conference on Multiphase Flow (ICMF). Toulouse, France. May 2025.

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Johannes Hansson
Gothenburg, May 2025

Acronyms

AI	artificial intelligence
CFD	computational fluid dynamics
DDES	delayed detached eddy simulation
DES	detached eddy simulation
DMD	dynamic mode decomposition
DNS	direct numerical simulation
HDD	hard disk drive
LES	large eddy simulation
LPT	Lagrangian particle tracking
ML	machine learning
NVMe	non-volatile memory express
POD	proper orthogonal decomposition
RAID	redundant array of independent disks
RAM	random access memory
RANS	Reynolds-averaged Navier–Stokes
rCFD	recurrence computational fluid dynamics
SSD	solid-state drive

Contents

Part I

Extended Summary

Chapter 1

Introduction

Particle deposition is a phenomenon that often adversely affects industrial and everyday systems such as soiling of cars, icing of aircraft, and ash build-up in boilers. Although it is a commonly occurring effect, there are still significant shortcomings in our ability to accurately model how these systems are affected when subjected to real-world working conditions. The basic principles of particle tracking are well known, and there are plenty of particle deposition models that account for the deposition and rebound behavior of the particles [1]. However, little is known about how these systems act when complex flows or large numbers of particles are introduced. This limitation is in large part due to the experimental difficulties and extreme computational requirements that are associated with deposition studies. For experiments, there are several challenges in measuring the behavior of individual soiling particles in a particle-laden flow. For numerical simulations, one of the main obstacles is the cost of running high-accuracy models for the extended periods of time required for particle deposition studies.

In this project we aim to evaluate the usefulness of using recurrence computational fluid dynamics (rCFD) [2] to generate time-extrapolated approximations of the carrier-phase flow fields for particle deposition studies. Simulating these flow fields is a major factor driving the extreme computational costs, so if this cost can be reduced, then many more types of deposition studies become computationally feasible. This thesis presents our implementation of the rCFD solver, numerical validation of the solver using the benchmark case of deposition on a cylinder, and finally, we explore time-dependent effects that influence rCFD database creation. In the second, upcoming, part of the project we aim to further develop the solver and validate it against more complex bluff bodies that more realistically represent industrial flow systems. We will also experimentally validate the solver using particle deposition experiments in wind tunnels.

Two papers are part of this thesis. Paper I focuses on the numerical validation of the newly implemented rCFD solver and the simulation methodology that was developed for this project. The paper presents a validation case of particle deposition on a cylinder. In the paper, we show how the deposition efficiencies on the cylinder can be reproduced using the rCFD-based solver at a fraction of the computational cost of the reference simulation methodology based on conventional computational fluid dynamics (CFD) with flow fields generated using the delayed detached eddy simulation (DDES) model. The paper also contributes new results for particle deposition efficiencies on the front and back sides of a cylinder, an area of literature that suffers from large uncertainties in the reported values.

In paper II we investigate the time dependence of particle deposition rates on the back of a cylinder. We find that the deposition rates are highly variable in time, with observed differences of up to a factor 27 in short-term deposition rates between low- and high deposition rate events for flow at Reynolds number Re = 6600. These fluctuations act on very long time scales, with fluctuations typically occurring on timescales of tens of vortex shedding periods or more. In the paper, we establish a correlation between the deposition rates and the cylinder base pressure. When the base pressure decreases, the deposition rate increases. Previous studies have linked the cylinder base pressure to changes in wake size and intensity of shear layer turbulent fluctuations, where lower base pressures correlate with smaller wake sizes and more intense turbulent fluctuations [3]. In the paper, we then determine that the deposition rates are influenced by the size and behavior of the wake, and that the base pressure can be used as an indicator for this behavior.

This thesis is organized into two parts. Part I presents an extended summary of the project and the research carried out so far. Then, part II contains the two articles that have been produced within the scope of the project. In part I of the thesis, the background of the project is introduced in chapter 2. Then, chapter 3 describes the simulation methodology and the mathematical models used. Some of the most notable numerical results from papers I and II are presented in Chapter 4. Finally, chapters 5 and 6 summarize the main conclusions so far, and introduce the main goals for the continuation of the project.

Chapter 2

Background

This chapter outlines the main motivations for this project and some of the underlying theory. First, in section 2.1, we describe one of the major industrial applications, soiling of sensors in the automotive industry. Then, section 2.2 introduces the main modeling approaches commonly used for describing soiling particles, the Eulerian and Lagrangian approaches. This project focuses on Lagrangian modeling, summarized in section 2.3. In addition to the Lagrangian particle tracking (LPT) modeling, an introduction to particle deposition mechanisms is presented in section 2.4, with the special case of deposition on a cylinder summarized in section 2.5. A comparison of simulation methods is introduced in section 2.6. Finally, an outline of the rCFD method is presented in section 2.7.

2.1 Sensor soiling

A key motivation for this project is the need to better understand particle deposition and soiling for applications in the automotive industry [4, 5]. Modern cars are becoming increasingly automated, with several new systems for active safety, driver assistance, and self-driving. In order to support these automated systems, a large set of new sensors is being installed in newer car models. Sensors work best when they are clean and not exposed to various soiling materials that can adversely affect their functionality. Unfortunately, sensors in natural environments are exposed to a wide range of contaminants, including rain, snow, dust, and mud. The contaminants will inevitably start to cover exposed sensors, causing inaccurate readings or potentially preventing the sensors from working altogether.

One of the major challenges facing automotive manufacturers is how to design sensor systems that are as resilient as possible against malfunctions caused by soiling. One of the simplest solutions is to manually clean the sensors when necessary, for example by requiring the driver to clean the sensors by hand. This is undesirable due to the additional maintenance that would be required. Another solution is to introduce built-in cleaning systems near the sensors that can be activated without having to involve the driver. However, this approach introduces additional complexity in an already complex car, further increasing production difficulties and cost. Instead, it would be best if the sensors could be kept from getting soiled in the first place. This would reduce maintenance costs while at the same time increasing reliability and safety. However, this approach requires more effort to design and an extensive understanding of the particle deposition and soiling processes involved.

There are two main branches when trying to understand the soiling mechanics, experimental and computational. The experimental branch is conceptually straightforward, where a given design is tested directly in the relevant environment. This gives the best results for the effects of soiling, but creating a new vehicle for each design iteration is slow and expensive. Instead, the computational branch is often used first, where soiling particles are modeled together with a CFD simulation of the air flow around the vehicle. This approach is simpler in the sense that no physical object must be created in order to generate results. However, accurately modeling the fluid flow and the soiling particles is still a major challenge, especially with limited computational resources.

2.2 Modeling soiling

Broadly speaking, there are two categories of methods for simulating soiling particles, Eulerian and Lagrangian methods [6, 7, 8, 4]. The fluid is often treated in an Eulerian framework, so we commonly refer to these multiphysics methods as Euler-Euler and Euler-Lagrange. Euler-Euler methods model the soiling particles as a continuum, whereas Euler-Lagrangian models model soiling using a collection of discrete soiling particles. The continuum description in Euler-Euler methods works well when the soiling particles have identical properties. The discrete particles in the Lagrangian description, on the other hand, are well-suited for describing dilute particle-laden flows where there are clear individual soiling particles with varying properties in the system, for example snowflakes or small suspended rain droplets with a size distribution. In this work we focus on Euler-Lagrange modeling due to the direct representation of individual soiling particles and straightforward description of particle inertia, a fundamental property for particles suspended in a flow.

2.3 Lagrangian particle tracking

The Lagrangian part of the Euler-Lagrange model used in this work, LPT, asserts that particles can be treated as point particles, provided that the particles fulfill a set of prerequisites [8]. The main requirement is that the particles must be small compared to the size of features in the carrier fluid flow. Although not required, a common additional assumption asserts that the particles are spherical. This second assumption simplifies modeling by neglecting the effects of particle rotation and shape. With these two assumptions, the fluid-particle forces can be approximated using the corresponding values for an equivalent sphere of the same size as the real particle. This greatly simplifies force calculations since forces do not need to be integrated over the entire surface of the particle. Also, the point-particle approximation enables the direct use of Newton's second law of motion when propagating the particles in the flow field.

The law is expressed as

$$\mathbf{F} = m\mathbf{a}, \tag{2.1}$$

where $\mathbf{F}$ is the particle force vector, m is the mass of each particle, and $\mathbf{a}$ is the acceleration vector. The force vector is expressed as a sum of several contributing forces, for example drag, lift, and gravity. Depending on the specifics of the carrier flow field, some of these forces may be negligible in magnitude and can be ignored without affecting the results. The particles in this work are small, non-Brownian, and significantly heavier than the carrier fluid. The dominating force component is then the drag force [7]. In addition, the particle Reynolds numbers are small, consistently less than unity, so effects of the lift force can be neglected [9].

The drag force is defined using

$$\mathbf{F}_D = \frac{1}{2}\rho_f \mathbf{u}_{\mathrm{rel}}|\mathbf{u}_{\mathrm{rel}}|C_D A, \tag{2.2}$$

where ρ_f is the fluid density, $\mathbf{u}_{\mathrm{rel}} = \mathbf{u}_f - \mathbf{u}_p$ is the relative velocity between the fluid ($\mathbf{u}_f$) and the particle ($\mathbf{u}_p$), C_D is the drag coefficient of a sphere and A is the projected area of the particle into the flow. The drag coefficient on a sphere is defined by [10, 11]

$$C_D = \frac{24}{\mathrm{Re}_p}\left(1 + \frac{1}{6}\,\mathrm{Re}_p^{2/3}\right), \tag{2.3}$$

where

$$\mathrm{Re}_p = \frac{\rho_f \mathbf{u}_{\mathrm{rel}} d_p}{\mu_f} \tag{2.4}$$

is the particle Reynolds number, with d_p representing the particle diameter and μ_f representing the fluid dynamic viscosity.

A common way of characterizing particle inertia is using the Stokes number,

$$\mathrm{St} = \frac{\rho_p U_\infty d_p^2}{9D\mu_f}, \tag{2.5}$$

where ρ_p is the particle density, U_∞ is the fluid free-stream velocity, and D is the cylinder diameter. Particles with large Stokes numbers have high inertia and are only weakly influenced by the surrounding flow field. These particles tend to travel relatively straight ahead, irrespective of what the carrier fluid is doing. Particles with small Stokes numbers have little inertia and are strongly influenced by the carrier fluid. These particles behave similarly to tracer particles, following the fluid flow almost perfectly.

In addition to being influenced by the carrier fluid, particles may also couple back to the flow fields or to other particles. The strength of this coupling is determined mainly by the particle volume fraction, the fraction of a given volume that is taken up by the particles [4, 8]. For very dilute systems, there are not that many particles that may influence neither the carrier flow fields nor other particles. Only the carrier flow fields affect the particles. Using this assumption simplifies the modeling of both the fluid and the particles, and reduces the computational cost of simulating the system. This is known as one-way coupling, typically used for systems with volume fractions up to about 10^{-6} [8]. For slightly more dense systems with particle volume fractions between 10^{-6} and 10^{-3}, particles start to influence the carrier flow fields, and two-way coupling must be used. Further increasing the particle volume fraction above 10^{-3} causes particles to influence each other so much that particle-particle interactions must be taken into account. This is known as four-way coupling and can significantly increase the computational cost if many particles are present in the system. When studying particle deposition on bluff bodies, one-way coupling is often used [4, 7].

2.4 Particle deposition

Particle deposition is a complex process in which several physical mechanisms interact [12]. First, the particles are brought close to the wall surface by an in-sweep in the carrier flow [12, 13]. This brings particles to an accumulation region close to the surface. Once they have reached this region, they may either continue towards the wall and impact it due to the inherent inertia in the particle, or they may slowly diffuse closer to the surface until they finally collide. Alternatively, they may be ejected by turbulent structures in the accumulation region.

A commonly reported particle deposition metric is the impact efficiency η. It represents the fraction of all particles that impact the object surface $N_{\text{deposited}}$, compared to the total number of particles injected in front of the object N_{injected}. Particle impact efficiency is defined as

$$\eta = \frac{N_{\text{deposited}}}{N_{\text{injected}}}. \tag{2.6}$$

Note that the impact efficiency depends on various particle properties, mainly particle Stokes number. Comparisons of η for different types of particles should therefore be made with caution.

Not all particle-surface impacts lead to deposition. Some impacts lead to rebounds that redirect the particle trajectory back into the flow, often losing some energy in the process. The impact and rebound behavior is commonly described using various context-specific deposition models [1, 14]. For simplicity, in this work we assume that all impacts lead to deposition. This works well for academic predictions of deposition rates, but would likely produce some degree of overprediction when used to describe the deposition behavior of real particles. The terms impact efficiency and deposition efficiency are therefore synonymous in this work.

There is a characteristic difference between impact efficiency on the upstream front side and the downstream back side of the cylinder [7]. On the front, impact efficiencies are highest for high-inertia particles with large Stokes numbers. On the back, only relatively low-inertia particles with small stokes numbers hit. Deposition statistics are therefore often classified into front- and back side impact efficiencies [7, 15].

Impact statistics reported in literature are commonly time-averaged or time-integrated, meaning that temporal information has been filtered out. However, as we investigated in paper II, there are time-dependent effects that cause particle deposition rates to fluctuate significantly.

2.5 Particle deposition on a cylinder

Particle deposition on a cylinder has become an important benchmark case when developing new computational methods for particle tracking. The case benefits from the simple geometry and complex wake dynamics inherent in the single-phase version of the system, while at the same time providing a realistic and industrially relevant flow system for particle deposition. There are multiple studies of particle deposition on this system, showcasing the significance of this particular benchmark case [16, 15, 1, 7, 17, 18]. Other simple bluff bodies are also commonly studied, such as square blocks and circular disks [19, 20].

In general, deposition on the front side of the cylinder is well-understood and relatively simple to predict. The flow fields exhibit only minor time dependence, and there are no complex flow structures that may influence particles in chaotic ways. Most published results agree on the deposition rates for a wide range of particle Stokes numbers [7, 15]. On the other hand, deposition rates on the back of the cylinder are much more difficult to accurately predict due to the complex wake structures that interact with the particles. Deposition rates reported in literature can in some cases vary by more than two orders of magnitude, depending on study [7, 15]. Such large differences indicate that there are still complexities that must be better understood for the back-side deposition to be accurately predicted and reliably modeled. Nonetheless, it is still a valuable benchmark case for testing particle tracking and deposition models due to the well-defined geometry and good availability of numerical and experimental data for the corresponding single-phase problem.

2.6 Fluid simulation methods and computational cost

Ideally, we would like to use high-fidelity computational methods for all fluid simulation studies. However, the most accurate methods we currently have available for the fluid flow, direct numerical simulation (DNS)-based methods [21, 7], have extremely high computational costs, especially for complex, industrially applicable, flows. In practice, only small-scale problems can be modeled using high-accuracy DNS [22, 23]. In addition to the high computational costs of the fluid simulation, long-term predictions of particle deposition require not only very fine temporal resolution, they also need fields to be generated for very long time intervals. The already computationally expensive simulations then become drastically more expensive.

Alternative flow simulation methods have been developed to reduce the computational cost associated with simulating the fluid flow. One approach, known as large eddy simulation (LES) [24, 25], models small-scale turbulence instead of resolving it, reducing computational costs, but unfortunately also accuracy. Another method, Reynolds-averaged Navier–Stokes (RANS) [26, 27], solves the time-averaged Navier-Stokes equations, further reducing computational cost and accuracy. There are also hybrid LES/RANS methods such as detached eddy simulation (DES) [28], which combine the LES and RANS methods. In DES, large scale structures are resolved using LES, and small-scale turbulence, especially near walls, is modeled using RANS. The study in paper I uses a slightly modified version of DES called DDES, which counteracts issues of grid-induced separation found in traditional DES, and also improves the handling of thick boundary layers.

However, even with these computationally cheaper methods for generating the flow fields, the costs for performing long-term fluid flow simulations are still extremely high. One strategy for counteracting this has been the development of various reduced-order methods. These methods reduce an originally high-dimensional problem to a lower-dimensional one that preserves the most important degrees of freedom. The signal can be decomposed into a set of modes that represent the flow field evolution using methods such as proper orthogonal decomposition (POD) [29] and dynamic mode decomposition (DMD) [30]. Unfortunately, methods based on POD suffer from instability problems for long time frames.

This method generates time-extrapolated approximations of periodic flow fields at a fraction of the computational cost of conventional CFD methods. In generating the approximations, a time-space trade-off is applied to the simulation methodology by replacing some of the computational cost with increased data storage requirements. Conventional CFD methods have high computational costs for generating new flow fields, but require no additional storage other than the storage required for saving the mesh and output files from the simulation. The rCFD method, on the other hand, has almost no computational cost when generating new approximations, but it requires storage space for the database of flow field snapshots. Additionally, it requires a preparation step to generate the flow field database using conventional CFD, which has both a computational and a storage cost.

2.7 The rCFD method

To be able to generate flow-field extrapolations for long time frames we turn to the rCFD method. At its core, the rCFD method represents a time-space trade-off. Conventional CFD simulations can be very accurate, but this accuracy comes at a significant cost in computational complexity. Flow fields for large, industrially applicable, cases can in many cases only be generated for a few short instants of fluid flow. Long-term simulations, such as those required for particle deposition, are completely unattainable. The rCFD method aims to overcome this limitation by identifying periodicities that are found in the time evolution of the flow system. A series of snapshots is saved from a conventional CFD simulation, and these snapshots, together with the identified periodicities, are used to construct a time series of extrapolated flow fields. Generating a set of extrapolated flow fields is computationally very cheap, but the database that stores these flow field snapshots requires some storage space. The method has then traded computational cost against storage space. For further details on the rCFD method, see section 3.3 and paper I.

Chapter 3

Methodology

In this project we use conventional CFD and LPT methodologies, as well as a newly developed rCFD-based simulation procedure. The CFD and LPT methodologies are summarized in sections 3.1 and 3.2. An overview of the rCFD method is presented in section 3.3. Since the rCFD method poses new challenges for available computational data management infrastructure, an outline of important considerations for computational performance is introduced in section 3.4.

3.1 Fluid flow fields

The particle deposition studies in this project are inherently time-dependent, so time-resolved flow fields are used for all simulations. The rCFD method is not sensitive to how the flow fields are generated, so any conventional solution method such as DNS, LES, or DDES can be used when creating the flow fields for the rCFD database. In this work, the investigation of rCFD in paper I uses DDES both for the reference simulations and for creating the flow field database. The conventional CFD study in paper II uses DNS. The simulations, both for the carrier fluid and the particles, are performed using the OpenFOAM software package [31].

3.2 Particle tracking and deposition

This project uses a mostly standard LPT methodology. However, the main difference is that particles are tracked not only in regular CFD fields, but also in the approximated rCFD flow fields described in section 2.7. Using precomputed flow fields from the rCFD database is in principle trivial, but in practice requires implementation of a small utility for loading flow fields from disk. In the OpenFOAM framework developed in this project, this problem is solved using a solver that loads the flow fields from disk and then runs the LPT using an existing particle tracking function object. In OpenFOAM, function objects extend the running solver by adding functionalities such as field computations, averaging, or particle tracking features.

An important addition to the standard LPT methodology is the introduction of a particle radius check for detecting particle-cylinder impacts where the particles just barely graces the cylinder surface. Commonly in LPT, impacts are registered when the center of mass of the spherical particles touches the surface of a wall, in this case the cylinder surface. However, many particle impacts on the cylinder occur at very shallow angles of incidence. The center of mass may then never come close enough to the wall for a collision to be registered, even though the outer shell of the spherical particle is, in fact, touching the wall. This collision mode is especially important for small particles with low inertia, as reflected by their low Stokes numbers. Failing to account for the particle radius in the collision detection mechanism would cause this mode of collision to be completely overlooked, leading to catastrophic underprediction of deposition rates for these low-inertia particles.

Particle statistics are gathered both as snapshots of particle positions at regular time intervals, and as discrete impact events when a particle deposits on the cylinder. This data is used to reconstruct particle trajectories and time-resolved deposition rates.

3.3 The rCFD solution methodology

The rCFD solver methodology developed in this project is composed of four simulation steps and two major software components. The four simulation steps are database generation, creation of the recurrence matrix, creation of the recurrence path, and finally solution of the particle tracks in the time-extrapolated flow fields. The software components are the main Python script for generating the recurrence matrix and paths, and a flow solver that reads the flow fields in the database, as indicated by the computed recurrence path.

The first step in the developed rCFD methodology, database generation, involves running a conventional CFD simulation and regularly saving flow field snapshots. These snapshots make up the rCFD database. Then, in the second step, creation of the recurrence matrix, the main Python script is used to pairwise compare all flow fields in the database. The set of pairwise comparison results correspond to the elements in the recurrence matrix. This matrix is then used by the Python script to generate the recurrence path, which describes a path through the database for the time-extrapolated flow fields. Finally, the flow fields are loaded by a small custom-built solver according to the recurrence path, and particles are then tracked in these fields.

The main software component that has been developed in this project is a Python script that generates the recurrence matrix and computes the recurrence path. It implements the core functionality of the rCFD time-extrapolation method. This script is mostly agnostic to the simulation software used to generate the flow fields, although some minor adjustments may be required to load and save data in the desired format. The second component is a new OpenFOAM solver that reads the flow fields from the flow field database in the order specified by the computed recurrence path, and provides the solver infrastructure required for using existing OpenFOAM particle tracking function objects. This custom solver is by necessity specific to the particular software package used for simulating the flow fields and particles. However, the functionality of this solver can be implemented in any major simulation software, so the methodology is not restricted to only OpenFOAM. Only minor additional effort is necessary to add compatibility with other simulation software.

3.4 Considerations for computational performance in the rCFD method

Since the rCFD method relies on precomputed flow fields, the performance of the data management infrastructure is crucial for overall computational performance. This infrastructure encompasses not only the storage hardware itself, but also database layout and access algorithms, file system organization, file cache, and additional hardware components such as random access memory (RAM).

Of greatest importance is the amount of available RAM compared to the size of the flow field database. If the entire database fits in RAM, then computational performance is generally good. However, if the database does not fit, then other algorithmic and hardware aspects become important. Algorithmic optimizations for computational performance must typically be tailored for each phase in the rCFD process. In terms of hardware, computational performance is better if the fields are stored on fast solid-state drive (SSD) or even non-volatile memory express (NVMe) devices compared to slower hard disk drive (HDD) or network storage. Systems such as redundant array of independent disks (RAID) can further increase data read performance over single-disk equivalents.

The first step in the rCFD workflow, database generation, is typically insensitive to the performance of the data management infrastructure. Here, computational performance is mainly dictated by the processors that run the CFD simulations.

The second step, generation of the recurrence matrix, consists of a large number of pairwise comparisons of flow fields. If the entire database does not fit in RAM, then the computational performance will decrease. One mitigation that limits this performance degradation is to make the comparisons in an order that minimizes the number of times that fields must be reread from slow storage. Other mitigation methods include limiting the spatial dimensions of the flow field database, mapping the loaded fields onto coarser meshes, or casting the fields to data types with reduced numerical precision.

In the third step, generating the recurrence path, an efficient data structure is necessary to minimize storage use and maximize data read performance. The exact details for how to achieve this are specific to each set of CFD and LPT software packages. OpenFOAM, as used in this project, stores flow fields and particle properties as files in time directories, with one directory for each stored time step. The rCFD database is then composed of a set of time-indexed directories that contain the flow field snapshots. A long-running particle deposition simulation will often run far longer than the length of the rCFD database. This means that the same flow fields will be used more than once. In the default OpenFOAM file structure this would mean that we need to duplicate flow fields that correspond to the same time instant in the database, drastically increasing database storage size requirements. However, by using symbolic links in the underlying file system, a type of database deduplication is achieved, while at the same time keeping the default OpenFOAM file structure. The rCFD case structure does not contain the actual database, but just a collection of symbolic links to the database. The links can be renamed and still point to the same physical file. With the symbolic links we can then generate an arbitrarily long time evolution of flow fields, but using only a negligible amount of extra storage. This solution also optimizes operating system file cache operations, meaning that computational performance is potentially improved as a positive side effect.

In the final step of the rCFD simulation method, the flow field sequence generated in step three is read one time step at a time, and particles are tracked in the loaded flow fields. If the database is larger than available RAM, then performance of the hardware storage system becomes crucial. The solver will need to continuously read the next flow field from disk, which is comparatively slow. The main mitigation that is specific to this step is to implement a prefetching mechanism to the OpenFOAM rCFD solver, or other simulation software as applicable. Prefetching is the process of loading data into faster memory before it is actually needed. Since the flow field progression is known beforehand, the computer can load data ahead of time. This can assure that when the simulation reaches a certain point in time, the required fields are already present in fast RAM, minimizing unnecessary waiting time.

In summary, the time-space tradeoff applied by the rCFD method represents a potentially outstanding reduction in computational cost for performing long-term particle deposition studies. However, the method requires advanced data management methodologies for achieving good computational performance when using large databases. Many of these methods have already been implemented, or can be implemented by further developing the currently available rCFD solver.

Chapter 4

Selected results

The main results of this project so far are presented in papers I and II. Paper I introduces the newly implemented rCFD methodology and solver, as well as an extensive validation case of the rCFD method when used for particle deposition studies. Some highlighted results from this work are summarized in section 4.1. Paper II presents an investigation of the time-dependence of particle deposition rates on the back of a cylinder, summarized in section 4.2.

4.1 Cylinder back-side deposition using rCFD

The main results from paper I are the particle deposition efficiencies, produced using both DDES and rCFD flow fields, as well as a comparison of the computational cost of the two methods. For the deposition efficiencies, we computed both the front- and back side deposition efficiencies separately. The front side deposition efficiencies are practically identical for all simulation methods (see figure 7 in paper I). The remainder of this section will focus on the back-side deposition efficiencies and the computational cost.

Figure 4.1 shows deposition efficiencies on the back of the cylinder obtained using a reference DDES simulation, as well as literature values from several studies. There are very few published studies on the deposition efficiencies on the back of a cylinder, so a few results for a square block and a circular disk are presented as well. Literature values are presented as markers and the reference simulations using the DDES flow fields are presented as dashed lines. The figure clearly illustrates a considerable spread in the reported deposition efficiencies on the back of the cylinder. For example, at $\mathrm{St} \approx 10^{-1}$ the reported deposition efficiency results span approximately three orders of magnitude.

Figure 4.2 represents a simplified version of figure 4.1, keeping only one set of DNS results from literature [7] and the deposition efficiencies computed using DDES flow fields. The figure also illustrates the deposition efficiencies obtained using the rCFD flow fields, presented as solid lines. The figure clearly illustrates how closely the deposition efficiencies obtained using rCFD match the deposition rates obtained using the reference DDES flow fields. It is also clear that the deposition efficiencies obtained in this paper closely match the published deposition rates using the DNS flow fields for $\mathrm{Re} = 1685$.

The results for deposition efficiency at Re = 6600 are different for the study in paper I and the literature values. This difference is explained by the extra dimension used in the three-dimensional simulations in paper I, compared to the two-dimensional simulations in literature. An additional rCFD particle deposition simulation was run in two dimensions, and then the computed deposition efficiencies overlapped closely (not shown).

A comparison of wall-clock run time for the different types of simulations is presented in figure 4.3. The left bar summarizes the required wall-clock time for a conventional CFD and LPT simulation of the flow field (blue) and particles (orange) on the computer cluster node used in the study. The computational cost of the rCFD method is divided into two main categories, "rCFD preparation" and "rCFD". The "rCFD preparation" bar represents the time needed to generate the rCFD database and compute the recurrence matrix. These steps are just preparation steps for actually running the particle tracking in the main "rCFD" step, represented by the middle bar. This bar represents the time it takes to run a particle tracking simulation using the time-extrapolated flow fields that were generated using rCFD. The computational cost is almost entirely due to the cost of simulating the particles. There is also a negligible cost for reading flow-field data from storage. The cost of simulating the particles is approximately equal in both the reference and rCFD simulations.

The division between "rCFD preparation" and "rCFD" also highlights one of the major advantages of using the rCFD flow fields for deposition studies. The preparation steps must only be run once for a particular flow system. Additional particle studies can be run using the same preparation step, virtually eliminating all computational costs except the particles themselves.

4.2 Time-dependent particle deposition

Paper II uses DNS simulations to investigate the time dependence of particle deposition rates. We showed that the deposition rates were highly variable in time, as illustrated by the orange lines in figure 4.4(a) for the Re = 6600 case and figure 4.4(b) for the Re = 10 000 case. We observed short-term variations as large as a factor 27 difference between low- and high deposition rate events for the Re = 6600 case. The fluctuations are very slow, occurring on timescales in the order of tens of cylinder vortex shedding periods or more.

In the paper we also show that the impact rate correlates with the cylinder base pressure, measured at the cylinder surface close to the rear stagnation point (blue lines in figures 4.4(a) and 4.4(b)). A decrease in base pressure leads to an increase in particle deposition rates, and vice versa. A decrease in base pressure has in previous studies been linked to a decrease of the wake size, as well as an increase in shear layer turbulent fluctuations [3]. The base pressure can therefore be used as an indicator variable for overall wake behavior. Consequently, we associate the time-dependent deposition rate fluctuations with the low-frequency modulations of wake size and behavior.

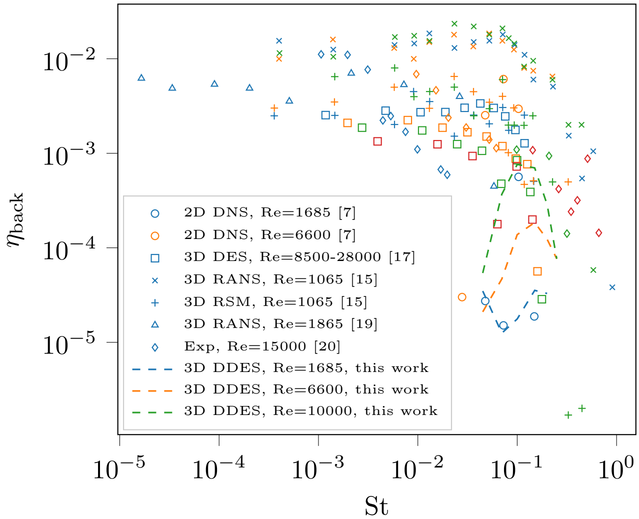


Figure 4.1: Back side particle deposition impact efficiencies as a function of the particle Stokes number. Literature values [7, 17, 15, 19, 20] are represented using markers and the CFD results from this study are represented by dashed lines. The graph includes literature values for a square block [19] and circular disk [20]. Figure from paper I.

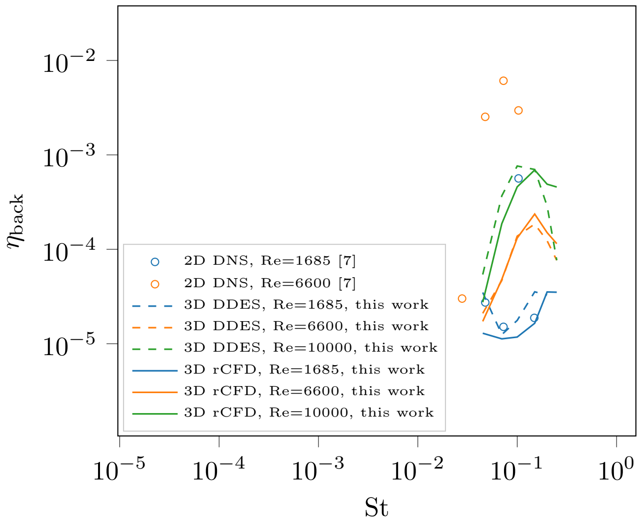


Figure 4.2: Back-side deposition results using DDES and rCFD, together with selected DNS results from literature [7]. Figure from paper I.

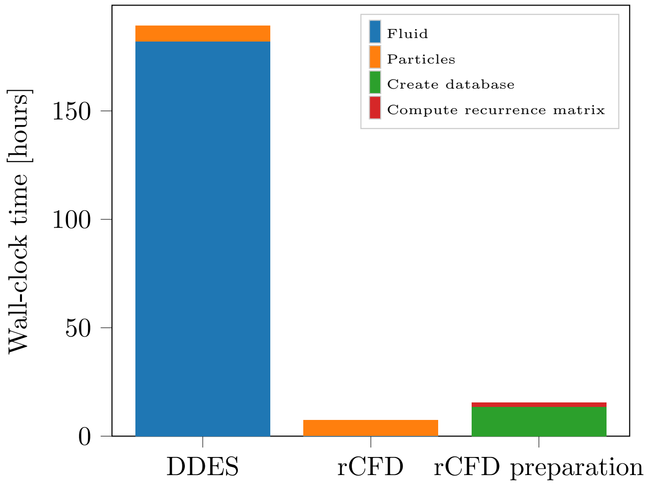
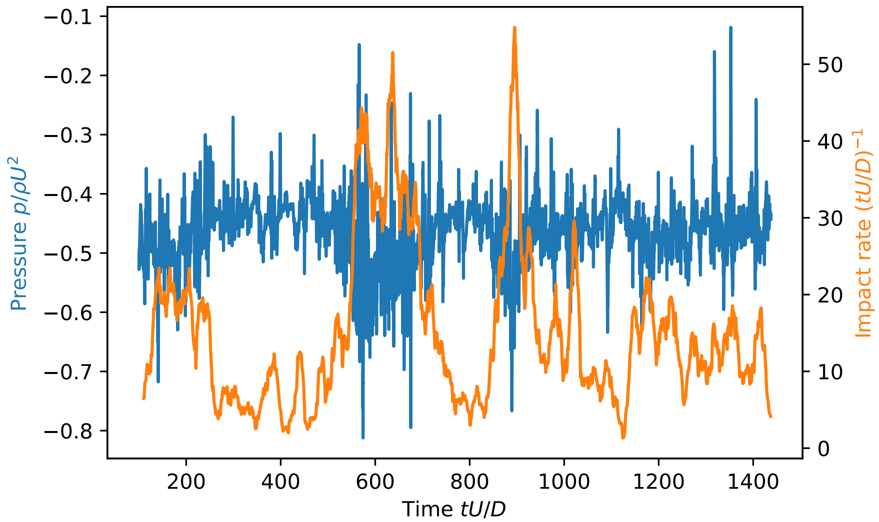
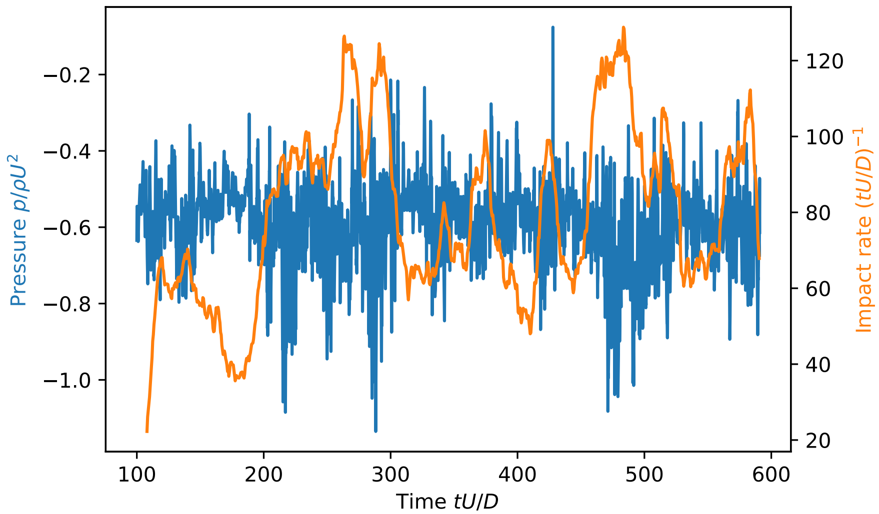


Figure 4.3: Computational performance of the DDES and rCFD methods, categorized by type of calculation. The latter method is divided into two phases, "rCFD preparation" and "rCFD". The rCFD preparation phase is only run once for each flow system, the rCFD phase can be run once, or several times for parametric studies. Time is measured in wall-clock time. Figure from paper I.



(a)



(b)

Figure 4.4: Base pressure (blue) and particle deposition rates (orange) for (a) Re = 6600 and (b) Re = 10 000. A drop in base pressure is almost immediately followed by an increase in particle deposition rate. Figures from paper II.

Chapter 5

Conclusions

In this project we are developing a particle tracking methodology for long-term soiling of bluff bodies with flow fields generated using the rCFD method. In the first part of this project we focused firstly on implementing the method and validating the solvers for the special case of particle-laden flow around a cylinder. Secondly, we investigated the time-dependent behavior of the particle deposition, which might affect the rCFD database generation process.

In the cylinder validation case presented in paper I, we demonstrated that the rCFD method can accurately reproduce particle deposition rates, both on the front of the cylinder, as well as on the back. Getting accurate deposition rates on the back is especially challenging considering the complex particle-wake interaction the particles experience before impacting the surface. It was not clear *a priori* that rCFD would be able to accurately predict particle deposition statistics. In the paper, we not only demonstrated that the rCFD method is able to approximate the complex flow fields in the cylinder wake, we also showed that the method can do this at a fraction of the computational cost of conventional CFD simulations. The results were achieved using a relatively small flow field database size of 3 vortex shedding periods, indicating that good long-term approximations can be achieved using relatively small initial datasets.

In paper II we sought to evaluate potential fluctuations in particle deposition rates for the cylinder case as a function of time. In the study, using conventional DNS, we showed that particle deposition rates are not constant, but rather fluctuate significantly with time. These fluctuations are an effect that, to the best of our knowledge, has not been observed before. In the paper we also show that the fluctuations are quite significant, with an observed difference of up to a factor 27 deposition rates between low- and high deposition rate events for the back of the cylinder. Such large fluctuations risk introducing bias into the rCFD database if not managed properly, potentially leading to significant over- or underprediction of real deposition rates. The fluctuations also pose significant challenges for other data-assisted methods that rely on flow fields as training data, such as artificial intelligence (AI), machine learning (ML), and similar. It will be crucial for all future data-assisted methods to be aware of this low-frequency effect to avoid using training data corresponding to only either high- or low extremes of particle deposition rates.

Chapter 6

Future work

The investigations in papers I and II highlight the potential of using rCFD for particle deposition studies, but also call attention to potential database bias issues that may arise if the flow field database is not carefully constructed. As a result, several additional questions must be addressed before the method, and the current implementation of the rCFD solver, can be reliably applied in more complex situations. For example, the simulation infrastructure has so far only been tested numerically for the benchmark case of particle-laden flow around a cylinder. One of the future objectives of this project is to experimentally validate the rCFD solver methodology for the cylinder case. There is particular interest in validating the solver for flows with higher Reynolds numbers, especially given the current scarcity of particle deposition results for high-Reynolds-number flows.

Additionally, we will also study more complex geometries to investigate and generalize the applicability of the rCFD method to other bluff bodies, for example a wedge or the Ahmed body. These geometries exhibit vastly different flow field structures, and serve as good benchmark cases for geometries that are similar to bluff bodies used in other academic and industrial applications.

Finally, in the project we aim to numerically investigate a fully industrially-applicable case of external flow around a car. Car manufacturers routinely simulate the aerodynamics of this system for short time intervals to generate predictions of aerodynamic performance. However, predicting long-term soiling patterns with conventional CFD techniques is not computationally feasible with currently available methods. We will explore the possibility of using existing aerodynamic simulations as the basis for the rCFD database, which can then be used to generate flow field approximations for particle deposition studies. Simulations of soiling can then be carried out with only a little extra computational effort. In addition to numerical investigations of the system, experimental validation of soiling in a wind tunnel will also be an important component.

Particle deposition in complex flow systems is generally very challenging, if not practically impossible, to simulate numerically using conventional CFD methods and realistic computational resources. However, given the potential for drastic reduction of computational complexity when using the rCFD method, a positive result in this project could establish a new, higher baseline for what is computationally feasible.

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Part II

Appended Papers

Paper I: Recurrence CFD for efficient predictions of long-term particle deposition on a cylinder

Paper II: Low-frequency wake modulation governs particle back-side deposition on cylinders