Data-Informed Modelling of Aerosol Resuspension under Aerodynamic Loads

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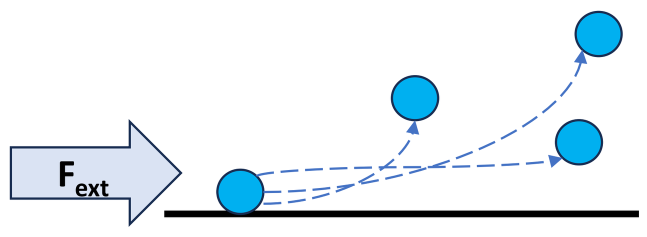
What is resuspension?

- Process through which **particles detach from a surface** to **become airborne**[1] through the action of **external forces**
- Ubiquitous applications:



Pollen, dust, sand, snow | Metals, fibres, pollutants | Virus, bacteria, bioaerosols | Pesticides, fertilisers | Brake, tyre & road/track wear

Problem statement

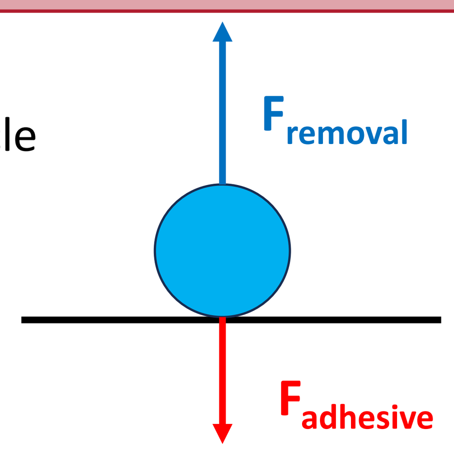
Current issues with existing resuspension model:

- Models are scarce and dated
- Mostly mechanistic and empirical
- Compromise between accuracy & computational cost
- Overall lack of data to perform numerical & analytical sensitivity

Need to investigate **novel solutions** to capture the complexity of the problem while enabling simpler and quicker steps towards resolution, combining accuracy and efficiency.
Can make use of **machine-learning techniques** to build on **numerical simulations** and **wind tunnel data** and enable useful **validation of existing models.**

Background

- **Rupture of the balance** between the forces moving the particle and those impeding its motion[1]
- Removal forces: unsteady fluid mechanics, mechanical & electrostatic forces, particle impaction and thermal gradients
- Adhesive forces: Van der Waals & electrostatic interactions, capillary forces, friction and chemical interactions
- 3 main resuspension modes: **rolling, sliding and lifting**



Resuspension mechanics: adhesive properties alter with complex interactions between

- **Particle properties**: size, shape (asperities), density, composition
- **Surface characteristics**: roughness, electrostatics, hydrophilicity
- **Flow conditions**: fluid velocity, Reynolds number and turbulence scale, boundary layer
- **Environment**: pressure, temperature, humidity

Some **existing models**:

- Detachment from surfaces with varying roughness in turbulent flow (Soltani et al, 1994 & 1995 and Ziskind et al, 1995 & 1997)
- RRH model: kinetic approach only considering lift and normal forces (Reeks et al, 1998)
- *"Rock'n'roll"* model[2]: rocking of a particle about an asperity (Reeks et al, 2001), later implemented by Biasi et al (2001)
- Recent model by Guingo and Minier (2008), enhanced by Henri et Minier (2014) has much greater complexity and requires more computational power.

Objectives

- Evaluation of the feasibility and accuracy of **resuspension experiments** in a **controlled laboratory environment** for varying **particle sizes, surface topologies** and **flow conditions**
- Investigation **of key parameters** influencing the resuspension mechanism and how they **interact** and **correlate** with each other
- Application of **numerical** and **Computational Fluids Dynamics (CFD)** methods to solve scenarios of increasing complexity and gather data
- Assimilation of **experimental** and **numerical data** into **machine-learning-based semi-empirical models** to achieve highly accurate **resuspension predictions** for a broad range of scenarios

Policy and Responsible Innovation

Policies:

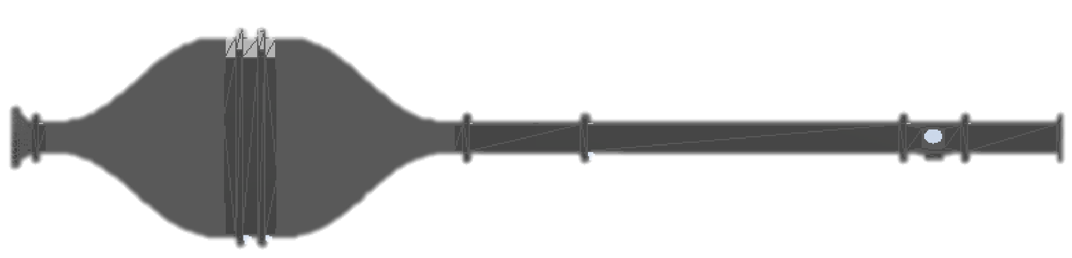
- **Health and safety regulations**: evaluate resuspension hazards (e.g. dust & fibres in factories, viruses in hospitals)
- Adjust **tolerance thresholds** for particles highly prone to resuspend
- Regulate industrial **accidents** and sanction **malpractice**

Responsible Innovation:

- **AI training data-use**: use own data or get consent to use 3rd party's
- Model application: unethical and harmful usage very unlikely
- NN and CFD methods **environmental impact**: very computationally intensive, thorough planning required to limit footprint

Methodology and techniques

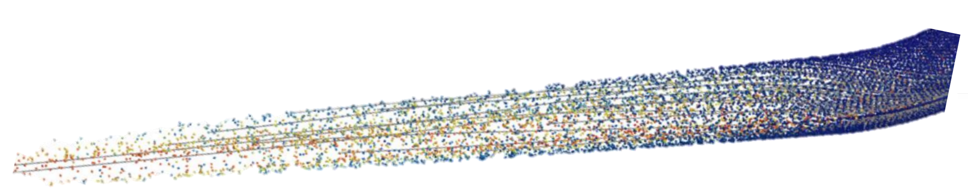
Phase 1: Experimental



3D printed wind tunnel, E. Neal [3]

- **Wind tunnel testing** to evaluate different resuspension scenarios
- Varying **particle sizes** and **surface morphologies**
- Variation in **fluid velocity** and **turbulence scale**
- Investigation of **time-varying effects**
- Instruments: **particle imaging** & **hot wire anemometry** to gather data (e.g. pressure & velocity fields, turbulence intensity, particle path, aerodynamic forces)

Phase 2: Numerical

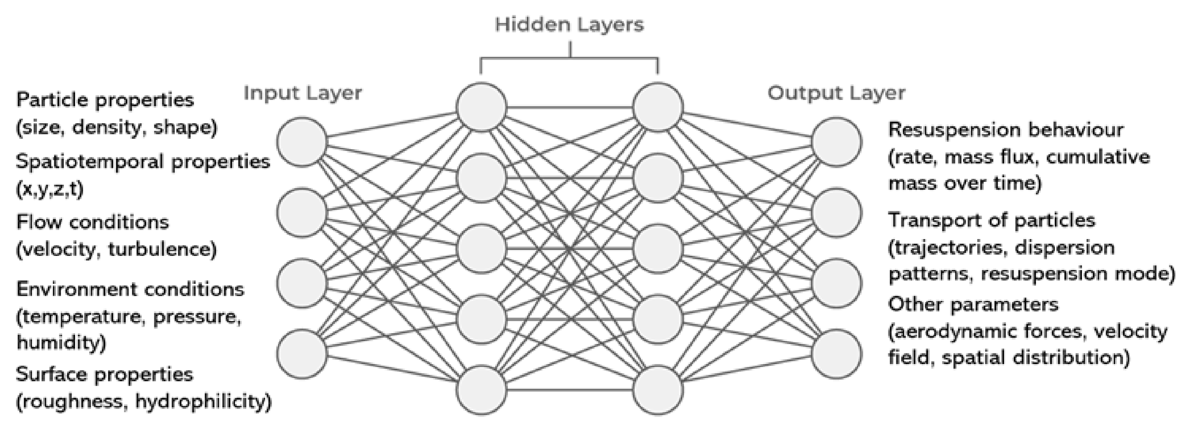


Lagrangian particle tracking CFD simulation using Star-CCM+

STAR-CCM+

- Numerical methods to investigate resuspension
- **Computational Fluids Dynamics (CFD)**: analyse and predict flow & particle behaviour for complex scenarios
- Definition of **complicated geometries** to perform very **realistic simulations** with real-life-like conditions
- Modelling of **other phenomena**: fluid-structure interaction, multiphase, electrostatics, thermogradients
- High spatial & temporal resolution
- Cross-validation of phase 1, generation of additional data

Phase 3: Modelling



- **Physics-Informed Neural Networks (PINNs)**[4]: universal function approximator
- **Reduced-order** models
- Highly **modular** and versatile
- Powerful **data-driven tool** to model resuspension in a simplified and physics-accurate way

Challenges

Data management:
- Measurement errors/noise
- Sufficient scope and frequency
- PINNs overconstraining

PINNs convergence:
- Complex model, many layers
- Multiple parameters to predict
- Lengthy computations, no convergence guarantee

Model interpretability:
- NN seen as a "black-box" tool
- Lack of transparency
- Path to solution and output reasoning is not always clear

Computational needs:
- PINNs and CFD lengthy and expensive to run
- HPC facilities required
- Extensive planning ahead

[1] W. C. Hinds, 'Adhesion of Particles', in Aerosol Technology: Properties, Behavior, and Measurement of Airborne Particles, John Wiley & Sons, Incorporated, 1999.
[2] J. C. Vincent, J. Hill, M. D. Walker, S. A. Smith, S. E. Smith, and N. E. Cant, 'Towards a predictive capability for the resuspension of particles through extension and experimental validation of the Biasi implementation of the "Rock'n'Roll" model', J. Aerosol Sci., vol. 137, p. 105435, Nov. 2019
[3] E. Neal, 'Understanding the Impact of Morphology on Particle Resuspension with a 3D Printed Wind Tunnel', presented at the Annual Aerosol Science Conference 2023, NPL, Nov. 17, 2023.
[4] M. Raissi, P. Perdikaris, and G. E. Karniadakis, 'Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations', J. Comput. Phys., vol. 378, pp. 686–707, Feb. 2019