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Particle Emission and its Mathematical representation using DEM

dokt. Sai Manoj Rayapureddy
Faculty of Transport Engineering
Department of Automobile Engineering
Vilnius Tech, Lithuania

Abstract

Replacing the conventional filters is associated with cost and reducing the emission of Fine particles that are less than 2.5µm are subjected to research. The convenient way of filtering the fine particles is through agglomeration and one such most predominant way is through acoustic waves. While very few research suggested the practical aspects of agglomerating the particles, in this research, we are mathematically evaluating the agglomeration effects on Particle parameters in the presence of Acoustic waves. Discrete Element Method is used in this process where Orthokinetic Interactions and Acoustic Wake effect are considered. The model is designed to have a smaller volume where particles are confined to a smaller volume due to the time involved in simulating larger volumes and higher particles.

Introduction

— PART 1

Problem

European Commission

Road transport is the largest source of air pollution in cities.

In 2018, more than 39% of NOx and 10% of primary PM2.5 and PM10 emissions in the EU came from road transport. It is estimated 300,000 premature deaths are caused by fine particulate matter annually.

In 2035, Euro 7 will lower total particles from the tailpipe by 13% from cars and vans, and 39% from buses and lorries, while particles from the brakes of a car will be lowered by 27%.

Although a significant reduction in fine particle matter is observed in the European Union by 37% between 2000 and 2020, emissions are now still considered to be at a harmful level

Hypothesis

Particulate filters are considered to be the most effective after-treatment methods due to its simple nature and have been widely used in commercial vehicles. These filters capture tiny particles that are released from the exhaust.

Most conventional mechanical filters use a dense layer of fibrous material to trap particles. The pores or spaces between the fibers determine the size range of particles that can be trapped. PM10 can be easily filtered through conventional filters with a collecting efficiency of 99%, but fine particles or PM2.5 escape through the filters.

If, in an effort to constrain smaller fine particles, the size of the pores in the filter are decreased, the soot accumulates over time and might cause filter clogging. This increases the exhaust back pressure of the engine leading to poor efficiency and fuel economy performance.

Objectives

Solution to reduce Particulate Emissions by using the existing conventional filters

Choosing the best simulation method to implement the found solution in the most appropriate way

Presenting Mathematical Model and testing

Significance of the Study

01 Research on new effective solutions such as the design of new combustion modes, use of blended fuels, and developing advances in particulate filters

02 Agglomeration is a technique in which smaller particles are excited through various sources and are forced to collide with each other to agglomerate and increase in size as a result of the formation of clusters

03 In a research conducted by Dong Zhou et al., they observed almost 10% improved efficiency in filtering PM2.5 particles when operated at 1400 Hz and 148 dB. Another experimental result shows that with an acoustic field of 21,400 Hz frequency, particles of size 10 µm are reduced by >90% and fine particles (0.3 µm) are reduced by ~45%

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Methodology

— PART 2

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Numerical simulation method

FINITE ELEMENT METHOD

Designed for problems involving continuous domains and is typically used for solving partial differential equations (PDEs) that describe the behavior of materials.

It's not inherently suited for simulating discrete, individual particles like those found in automobile exhaust emissions.

DISCRETE ELEMENT METHOD

Designed for simulating the dynamics of discrete, individual particles or grains and their interactions with each other.

The particles released from automobile exhaust are often very fine and may behave differently from larger, solid particles that DEM is designed to model.

COMPUTATIONAL FLUID DYNAMICS

CFD is well-suited for modeling fluid flow, including the transport of particles suspended in air.

It is ideal for capturing the interaction of sound waves with the air and the resulting fluid dynamics, including the pressure gradients and flow patterns generated by the sound waves.

Discrete Element Method (DEM)

In this research, Mathematical equations are determined for the simulation of Acoustic Agglomeration which needs each particle to be considered as an individual, discrete element.

The use of discrete elements in simulations allows for a more detailed and accurate understanding of particle-particle interaction than any other numerical simulation technique.

The movement of these individual elements, its influence on the movement of other elements, and the physical forces between them are considered.

By studying individual characteristics and the interaction between the particles, it is possible to estimate the agglomeration effect on a large scale.

Predominant first-order effects that enable the agglomeration of 2 particles in a system

ORTHOKINETIC COLLISIONS

Orthokinetic interaction is the interactive agglomeration process formed as a result of the direct collision of particles of different velocities.
Particles with different sizes act differently in the system due to their difference in inertia.
The primary drawback of this particular interaction is that it cannot be applied to particles with similar shape and sizes

ACOUSTIC WAKE EFFECT

AWE is a particle interaction process in which the acoustic wake causes a reduction in pressure behind the forward moving particle.
If another particle follows this wake, it would be experienced with a drag reduction and moves with an accelerated speed towards the leading particle, causing agglomeration of the 2 particles

At low frequencies particularly for medium-sized particles, Orthokinetic Interaction forces are found to be more applicable and Acoustic Wake Effect is found to dominate at higher frequencies for particles of different size

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Mathmeatical model of the Study

— PART 3

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Lagrangian approach

VARIOUS RECENT RESEARCH WAS SUCCESSFUL IN STUDYING THE BEHAVIOUR OF PARTICULATE SOLIDS USING THIS APPROACH

Considering the inter-particle forces (Orthokinetic Interactions) and external forces like Acoustic Wake Effect as the additional forces acting on the particle.

$$m^{*}\frac{d}{dt}\left(\frac{dx}{dt}\right) = F_g + F_{interparticle} + F_{external}$$

Gravitational force is determined by, $F_g = m^{*}g$ where $g = 9.8\ m/s^2$

Mathematical Model

Considering the cohesive and adhesive behaviour of particles, one common cohesive contact model - Linear Cohesion Model is chosen over Hertz-Mindlin model to calculate the inter-particle or Orthokinetic Interaction force

$$F_{interparticle} = \eta * m * v_{rel} + F_{cohesion}$$

where:

η = orthokinetic interaction coefficient.

m = mass of the particle.

v_{rel} is the relative acceleration between particles.

The cohesive force between particles can be represented as the following using linear cohesion model

$$F_{cohesion} = A * \Delta s * \alpha$$

where:

A = contact area between particles.

Δs = overlap or separation distance between particles.

α = cohesive strength

Mathematical Model

Acoustic Wake Effect in terms of drag force is expressed as:

$F_{external} = 6*\pi*\mu*r* v_{rel}$

where:

μ = dynamic viscosity of the fluid.

r = radius of the particle.

v_{rel} = relative velocity between the particle and the fluid.

The above simplified equation is generated assuming Stokes flow and ignoring complexities associated with fluid-particle interactions.

Final Resultant equation:

$$m*\frac{d}{dt}\left(\frac{dx}{dt}\right) = (9.8*g) + (\eta*m*v_{rel} + A*\Delta s*\alpha) + (6*\pi*\mu*r* v_{rel})$$

Simulation Result of the Study

— PART 4

Computational Results

SIMULATION IS CONDUCTED TO TEST THE TENDENCY OF PARTICLES UNDER THE APPLICATION OF SOUND WAVES

- The test consists of 10 particles that are randomly generated with different sizes.
- Each such generated particle is assigned predetermined properties such as mass, shape, and other physical properties. These properties define the particle interaction and its environment.
- The sound intensity of the acoustic field is maintained at 140 dB throughout the test time.
- The algorithm of the DEM determines which particles are in contact and calculates the forces acting on those particles. Besides the gravitational and inter-particle interaction forces and other normal forces, external forces like the Wake Effect can be applied to the simulation.

Results

All 10 particles are subjected to sound waves at 3 frequencies (2 kHz, 3 kHz, and 5 kHz) and the exhibited agglomeration of particles is recorded.

Table. Name and Size of the generated particles

Particle Number	*Particle Name*	*Particle Radius (m)*
1	P1	1.024E-09
2	P2	5.036E-08
3	P3	1.987E-08
4	P4	1.309E-08
5	P5	3.522E-09
6	P6	1.256E-06
7	P7	3.111E-06
8	P8	3.284E-06
9	P9	1.807E-08
10	P10	1.010E-06

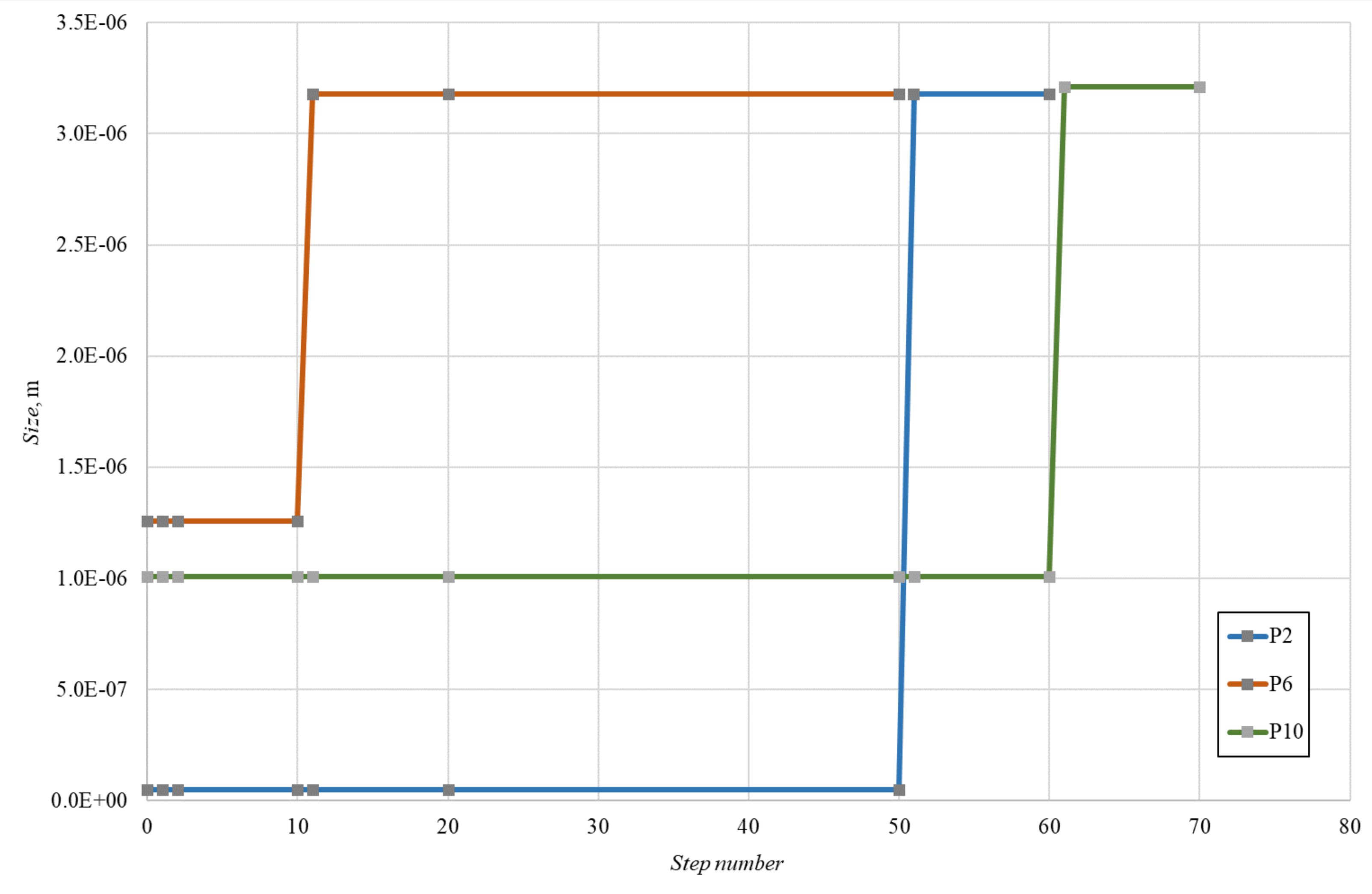

Figure. Agglomeration of particles at 2kHz

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Conclusion

— PART 5

PM2.5 are a potential threat to human health and the environment.

Orthokinetic collisions and Acoustic Wake Effect are the considered primary first-order effects that enable the agglomeration of particles.

Considering the limitations of other numerical simulation techniques in understanding the particle-particle interaction, the discrete element method is chosen over finite element methods or computational fluid dynamics.

Theoretical Model of AA which is developed from the law of motion considering all the forces (gravitational, interparticle, cohesive, and external) acting on the particle.

Study highlights

The simulation consists of 10 particles that are randomly generated with a wide range of sizes (between 1.010E-06 to 3.522E-09). They are subjected to 140 dB of sound intensity of the acoustic field.

Three particles agglomerated at 2 kHz, and only one particle agglomerated each at 3 kHz and 5 kHz.
This may be because, in the field of high frequency, the tendency of particles getting more excited and exiting out of the testing area early increases, decreasing the chances of particles colliding with each other and agglomerating inside the boundary condition.

Agglomeration of Particle 6

Occurred at all 3 frequencies, is found to occur earlier with an increase in frequency.

2kHz - 11th step
3k Hz - 9th step
5k Hz - 8th step

This leads to an estimated understanding that with an increase in frequency, the particles have a higher chance of agglomerating faster.

Thank you for your attention

QUESTIONS OR SUGGESTIONS??