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Review

Recent Advances in Modeling of Particle Dispersion †

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Abstract: Particle dispersion is an important research area as this provides insight into how a particle behaves, how long the particle will fall, how far the particle will travel away from the source, and its concentration at a particular time and point of location. In this review paper, different models used to study the dispersion of particulate matter are explained and compared. The mechanism and factors that affect the dispersion of particles are discussed. Applications of the atmospheric dispersion model are also given. Moreover, the topics sufficiently lacking in the literature and insight into further areas that should be improved are discussed.

Keywords: Fluid-Solid Interaction; Particle Dispersion; Lagrangian; Eulerian; Gaussian

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1. Introduction

When a solid and a liquid combine, the solids clump together. These big clusters of particles may cause the liquid to disperse unevenly. Due to how little they are, we might not be able to look at the materials and see the enormous clusters. We can determine the sizes of your particles by putting them through a particle analyzer. We can confirm that the grouping of particles may still be too large based on the range in which the particles fall.

In regulatory and epidemiological contexts, modeling the dispersion of air contaminants is crucial. Even though most modeling ideas originated in the 1980s, dispersion models have been optimized and improved since then. Modeling techniques must be used with care to quantify component interactions. Significant propagation patterns of the variables can be captured by the quantified interactions, which can improve comprehension of the system and recognize the essential connections and elements that shape the system's behavior. Applications using fluid-solid interaction (FSI) entail the integration of the structural mechanics and fluid dynamics fields [1]. Several new models, like computational fluid dynamics, have also been developed. Moreover, the accuracy of the data acquired is continuously being enhanced by next-generation representations [2].

2. Theoretical background

2.1. Modeling air quality

The atmospheric mechanisms that spread a pollutant generated by an origin are described by dispersion modeling, which uses numerical equations. The levels at specific downstream receptor sites can be predicted using a dispersion model according to emissions and meteorological parameters. The National Ambient Air Quality Standards (NAAQS) and other regulations are observed using these air quality algorithms. Modeling dust dispersal from extraction processes is based on four quantitative techniques: the Lagrangian Model, Eulerian Model, Gaussian Model, and Box Model.

2.1.1. Lagrangian Approach

According to the Lagrangian method, the fluid is thought to be made up of several fluid particles, and each fluid parcel is followed as it moves to measure how its properties change over time.

$$V = V(t), \tag{1}$$

Imagine being in a car and seeing the vehicle's displacement, speed, and acceleration over a period. Because it follows a material (fluid) particle, a Lagrangian characterization is also known as a material description. This approach uses the qualities as a function of time to characterize the fluid motion.

In terms of atmospheric dispersion, a moving reference grid based on the wind direction and the general direction of plume flow is used by the Lagrangian model to compute the dispersion of plume parcels. The reference grid follows the plume as it moves, and the movement of the plume is modeled using an arbitrary walking approach. The likelihood function is constructed from site-specific meteorology, distribution of particle sizes, and particle density. Despite its dynamic character, the Lagrangian model has limitations [3].

The Lagrangian model is based on the Advection-Diffusion equation. The equation called advection-diffusion is a simplified version of the Navier-Stokes equation. This equation illustrates the particle motion that is affected by the air movement and diffusion that is turbulent. The left-hand side of the equation represents concentration change in a localized area at a point in time, while the letter Q represents the emission rate. Moreover, the terms, without the k constant, on the right-hand side of the equation denote the movement in three directions, x, y, and z, caused by the average wind speed. Lastly, the three factors with the k constant depict the movement caused by turbulent motions. The k constant means the coefficient of diffusion [3].

2.1.2. Eulerian Approach

In Eulerian analysis, measurements are made at a predetermined fixed location in space, where an observer at a particular location's concentration as a function of time is described. "Field description" also refers to the Eulerian consideration or description. The Eulerian approach never concentrates on specific fluid portions; instead, it studies the characteristics of the fluid as it passes by a specific fixed point.

The fluid parameters consequently become a function of space and time in Eulerian analysis. The z represents the vertical axis which typically denotes height or pressure.

$$V = V(x, y, z, t) \tag{2}$$

In atmospheric dispersion, the difference between the Eulerian and Lagrangian models is that the former uses a fixed reference grid. In contrast, the latter makes use of a moving grid. In contrast to the Eulerian model, which tracks a static grid as the pollution plume passes by, both models track the movement of pollution plumes over time [4].

Like Lagrangian models, the advection-diffusion equation is also the mathematical equation on which the Eulerian model is typically based. However, the method by which the two models simulate is different. Lagrangian models simulate the movement of particles to a frame that is moving with the average stream, akin to a person moving simultaneously with the particles. Because of this, the forward and backward routes can be generated, which can aid in visualizing the matter's starting and end points in the atmosphere.

Both the Eulerian and Lagrangian models are versatile. The two models can be used in different mixtures, conditions of the system, the area of the land, and the heights and depths of the land. These two models have an average of 1 kilometer to 100,000 kilometers resolution of spaces. Another configuration of Eulerian and Lagrangian models is a model that uses Computational Fluid Dynamics as a basis. Computational Fluid Dynamics offers a solution to the Navier-Stokes equation. Complicated terrains or simulation that would need a scale close to real-life proportions is suitable for Computation Fluid Dynamics. However, Computational Fluid Dynamics needs an enormous amount of data, unlike other models, to achieve this.

2.1.3. Gaussian Model

Gaussian dispersion models assume that the statistical distribution of pollutants is typically distributed. The two-dimensional (y and z) Gaussian plume grows over time. The following conditions must be true for the emission and atmospheric conditions: no chemical reactions must occur, and wind speeds must always be equal to or greater than 1 m s^{-1}. These conditions are all prerequisites for Gaussian plume models. Gaussian models are often applied when simulating the propagation of buoyant pollutants in air plumes. The commonly employed model is as follows:

$$X = \frac{Q}{2\pi\mu_s\sigma_y\sigma_z}\left[\exp\left\{-0.5\left(\frac{y}{\sigma_y}\right)^2\right\}\right]\left[\exp\left\{-0.5\left(\frac{H}{\sigma_z}\right)^2\right\}\right] \tag{3}$$

where X denotes the hourly concentration at downwind distance; μs is the mean wind speed at pollutant release height; Q is the pollutant emission rate; σ_y is the standard deviation of lateral concentration distribution; σ_z is the standard deviation of vertical concentration distribution; H is pollutant release height (stack height); and y is the crosswind distance from source to receptor.

Equation 3 has a steady state assumption. The equation estimates the concentration at any point in the direction of the source in which the wind is blowing. This equation also assumes the Gaussian distribution of particulate matter in the direction in which the wind is against the line of travel.

There are two Gaussian models: Gaussian plume and Gaussian puff models. The Gaussian model that comprises a permanent point is a Gaussian plume. A Gaussian model contains the equation encapsulated in the Lagrangian model. A Gaussian puff model breaks a continuous plume into individually separated and distinct packets of particulate matter. In this model, the concentration of particles can be traced back to the puff that contributed to the bulk of the particles.

With point source emissions, the Gaussian plume model is among the most popular and relies on employing empirical factors (sigma's) as a function, analyzing the transit and diffusion of the air pollutant particle of the atmosphere's stability. Environmental permitting processes frequently rely on Gaussian plume models, such as the Industrial Source Complex (ISC), AERMIC Model of AERMOD software, and CALPUFF, developed by the United States Environmental Protection Agency (US EPA), and the Atmospheric Dispersion Modeling System-Urban (ADMS-Urban), developed by Cambridge Environmental Research Consultants (CERC). Thus, although AERMOD software has superseded the ISC model, the latter is still widely utilized. This can be explained by the lack of or inaccessibility of input data needed by AERMOD software and other more complex models [5].

Among the inputs are the pollutant release rate, release height, wind speed (at the reference height, frequently the height at which emissions are released), mixing/inversion height, and the vertical and horizontal dispersion variables. Additionally, the plume's rise or fall can be modeled. The plume is expected to quantitatively reflect from the ground or the upper boundary layer of air when it reaches these surfaces. This may eventually give the erroneous impression that contaminants are collecting at ground level, which the model can consider [4].

2.1.4. Box Model

The approach for modeling air quality that is the simplest is the box model. The box model portrays the airshed as a straightforward box with uniformly concentrated contents. Following is the model that is typically applied:

$$\frac{dCV}{dt} + uC_{in}WH - uCWH = QA \quad (4)$$

where C is the concentration of pollutants throughout the box; C_{in} denotes the pollutant concentration entering the box; Q is the pollutant emission rate from the source per unit area; V is the volume of the box; A is the horizontal area; W is the box width; H is box height (mixing height); and u is wind speed normal to the box.

2.2 Modeling particle-particle interactions on dense solid-liquid suspensions in stirred vessels

Solid-liquid suspensions are widely found in industrial manufacturing operations. Both liquid-particle and particle-particle interactions affect how the solid-liquid suspension behaviors behave. This study examines the importance of particle-particle interactions in solid-liquid mixing vessels using a Eulerian-Eulerian model to define the dynamics of the suspension. Using a modified version of the kinetic theory of granular flow (KTGF), solid pressure and viscosity calculations are made while considering the impact and friction of coarse particles. Semi-empirical models are compared to the expected solid phase holdup and velocity. The effects of various essential model parameters are also examined. The multi-fluid model's robustness is confirmed by comparing computational fluid dynamics simulations with experimental data, demonstrating an acceptable agreement level. The suggested model is then used to explore the significance of particle-particle interactions by looking at the effects of particle size and solid loading. The simulation findings reveal that particle-particle interactions can alter suspension properties in the case of oversized particles. Solid–liquid suspensions in agitation vessels are essential for crystallization, polymerization, catalytic reactions, and mineral and water treatment. CFD simulations have been used to predict the hydrodynamic characteristics of solid–liquid two-phase flows, leading to insights into particle concentrations and velocity distributions. However, accurately simulating the suspension behaviors in stirred tank reactors is still challenging.

The Eulerian–Eulerian multi-fluid method considers solid particles as continuous phases. Particle–particle interactions can be considered through the kinetic theory of granular flow (KTGF) model. Research has shown that the roughness of particles exerts a significant effect on stress and particle rotation. Non-ideal particle–particle collisions are modeled based on the restitution coefficient. Most of the proposed KTGF models have been incorporated into CFD models for numerical simulations of hydrodynamics ingas–solid systems and solid–liquid suspension systems. The obtained predictions quantitatively agreed with experimental data.

Brucato et al. (1998) and Ranade's group (Khopkar et al., 2006, Sar Deshpande et al., 2010) evaluated the role of turbulent dispersion in predicting solid–liquid suspension quality. Feng et al. (2013) developed an explicit algebraic stress model (EASM) for simulating liquid–solid two-phase turbulent flow in stirred reactors. Hosseini et al. (2010) b developed a CFD model to investigate the solid–liquid mixing quality under different conditions. Montante et al. (2007) simulated the dilute solid re-suspension in a stirred reactor with multiple impellers. Tamburini et al. (2009) studied the dynamic evolution of solid–liquid suspensions by transient and steady-state simulations.

They developed an Eulerian-Eulerian multi-fluid model to predict suspend ability, critical agitation speed, and solid phase holdup. Blais et al. (2016) introduced a CFD-DEM coupled model to simulate viscous suspensions, consistent with experimental observations. They also investigated the influences of particle properties and mixer characteristics on viscous solid–liquid mixing.

This study developed an effective Eulerian–Eulerian model that incorporated the KTGF to investigate the effects of particle–particle interactions on the quality of solid suspensions. The modified CFD-KTGF coupled model was applied to simulate the dense solid re-suspension and studied the influences of particle size and loading [6].

2.3 Modeling particle dispersion in wall-bounded turbulent flows

Particle dispersion and deposition in a fully developed turbulent channel flow are investigated using direct numerical simulation (DNS). Results are compared with experimental measurements and numerical benchmark solutions. Two scenarios of fully elastic and no-rebound (trap-wall) collisions are considered. At lower Stokes numbers, the deposition velocity of the downward channel flow is higher than the upward flow. In comparison, at higher Stokes numbers, the upward flow has a higher deposition rate but a lower near-wall particle concentration. Understanding the physical mechanisms which affect particle motion in turbulent flow is essential for accurate predictions of turbulent quantities of particles. Inter-particle and particle-wall collisions have been shown to affect particle dispersion in wall-bounded turbulent flows significantly.

The impacts of turbulence, inter-particle collisions, and particle walls were examined in this study. Using a computational model of fully formed, turbulent flows loaded with particles of different mass loading ratios, collisions on particle dispersion are examined. Using the Reynolds-averaged Navier–Stokes (RANS) equations and a low Reynolds number k–turbulence model, the conventional method is utilized for the carrier-fluid flow field solution and the stochastic separated to solve the dispersed-phase (i.e., particle) flow field, flow model is used [7].

2.4 Modeling particle deposition and dispersion

A study investigated particle dispersion and deposition in a room using a novel hybrid RANS/LES turbulence model inside the Multi Relaxation Time (MRT) Lattice Boltzmann Method (LBM). For the hybrid RANS/LES technique, the LES model was used to evaluate the rest of the domain inside the confines of the LBM, while the RANS model was used to simulate the near-wall region. When RANS was used, the k - turbulence model was utilized in the near-wall layer. Particles with sizes ranging from 10 nm to 10 m were studied to replicate particle deposition and dispersion in space. Particle dispersion and deposition simulation results revealed that the present hybrid method's predictions were comparable to prior LES-LBM predictions. In addition, compared to the k - model, the predictions of the hybrid model for particle deposition and dispersion were more in line with the outcomes of LES simulations.

The Lattice Boltzmann Method (LBM) is a computational model simulating turbulent, multi-phase, and particulate suspensions. The Lattice Boltzmann Method (LBM) is a recent, efficient, and valuable computational technique that has drawn the interest of more researchers from many fields. LBM has been used to simulate single-phase flows, multi-phase flows, turbulent flows, particle flows in porous media, and multi-phase flow suspensions during the previous 20 years. The most popular technique for modeling interior air flows is the Reynolds-Averaged Navier-Stokes (RANS) equation in combination with a turbulence model [7].

2.5 Typical mixing behaviors of gas-solid-liquid flow in a rotary drum

In engineering industries, especially chemical engineering, the solid-liquid rotary drum method has a significant role in liquid-solid materials, like mixing. These drums involve complex multi-phase gas-solid-liquid flows, encompassing phenomena such as slipping, slumping, rolling, cascading, contracting, and centrifuging. The inner wall of the drum causes particles to lift through frictional forces, leading to the creation of a passive zone. As the particles reach a certain height, they slide down under the influence of gravitational force, forming an active zone. An optimal balance between mixing performance and energy costs is paramount in effective drum design and process optimization. Developing a knowledge and understanding of gas-solid-liquid flow and particle mixing characteristics within the rotary drum is essential to achieve this balance. This understanding will provide valuable insights into the dynamics and behavior of the system, enabling improved drum design and enhanced process efficiency.

A study focused on the development of a coupled Computational Fluid Dynamics-Discrete Element Method-Volume of Fluid (CFD-DEM-VOF) model to investigate the flow and mixing performance of the three phases (gas-solid-liquid) within a partially filled rotary drum. The primary objective is to analyze the effects of rotating speed on the system. The model is validated, and various aspects of the system are comprehensively observed. The study covers the transverse gas-liquid flow, voidage (fraction of volume occupied by gas or liquid), particle flow pattern (including active depth), particle velocity distribution, solid residence time, and particle mixing and dispersion. Higher rotating speeds lead to deeper active zones, enhanced mixing, and improved particle dispersion. Furthermore, liquid in the system contributes to a greater active depth, longer solid residence time in the active zone, and reduced contact force between particles [11].

2.6 Particle dispersion of solid-liquid characteristics

In mineral processing, Solid-Liquid fluidized beds (SLFB) are often used in settling velocity and were applied in leaching, washing, and particle size classification. Solid-Liquid fluidized beds (SLFB) express better phase segregation and mixing, which depend on particle diameter, difference of density, and slip velocity because of complex interactions between solid and liquid—a diffusion-like parameter known as the dispersion coefficient is frequently utilized to understand the hydrodynamics of SLFB.

The degree of segregation is mainly determined by the particle size and density ratio, which decreases as the fluid’s surface velocity increases. This study uses the segregation and mixing behavior of SLFBs (Solid Liquid Fluidized Beds) and the dispersion coefficient to describe these properties. Due to limited particle interaction and mixing, the particle dispersion coefficient becomes negligible when the bed is entirely segregated. This causes a rise in the particle dispersion coefficient, indicating improved mixing inside the particle. The model for the dispersion coefficient is consistent in diffusion coefficient specification and integrates the mean free path of collision and the gap fluid velocity. For both mono and multi-particle systems, it optimizes the model using experimental data spanning a wide range of particle sizes (0.39 to 23 mm), liquid superficial velocities (0.0009 to 0.6 m/s), and Reynolds numbers (4 to 2820). This study uses a one-dimensional convective-diffusive numerical model to simulate mixing and separation behavior in a binary SLFB system [12].

Atmospheric dispersion modeling can also be used in risk assessment. In a study conducted by [13], the trajectory of ash fall is examined. In this paper, the particle shape is studied as an essential parameter in the particulate matter dispersion, as numerous literatures have only considered spherical particles. It was found that the shape of the particle impacts the trajectory of the particle, especially if the diameter of the particle is greater than 1 to 3 micrometers. Particles with a sphericity of 0.5 or less move 44% farther than spherical particles. This is because of the low velocity of sedimentation in particles that are smaller in size compared to vertical velocity in the atmosphere, which is turbulence and horizontal movement of the wind. This conclusion is supported by [14]

Particles with a 0.1 to 100 micrometers diameter travel farther from the source. Moreover, the velocity of particles 100 micrometers in diameter is 5 magnitudes greater than particles with smaller diameters. Smaller particles fall slower and move up to 5 magnitudes farther than particles with bigger diameters. Thus, it was concluded that particle shape, sphericity, and density significantly impact the mass loading prediction of particle dispersion [14].

3. Research Gaps and Future Outlook

Particle dispersion modeling has a lot of various applications. This includes following the trail of movement of particulate matter, which can be challenging since there are many factors to consider, such as the particle's inertia, gravitational pull, and continuity effects. Tracking the particle movement would be more challenging if done in actual conditions. Currently, the standard methods to study the dispersion of particulate matter in turbulent flow are the eddy interaction model, Monte-Carlo method, and random walk models. The mentioned methods are beneficial in understanding the system behind inertia and the effect of crossing the direction of movement of particles. However, these methods often encounter convergence problems as numerous calculations in trajectory are a prerequisite. Furthermore, the eddy interaction model gives inaccurate results in modeling particle dispersion in turbulent regimes. This problem is also encountered in random walk methods such as Markovian [15].

Another application of atmospheric dispersion modeling is the analysis and assessment of risk [16] conducted a study on the liquefied natural gas dispersion once an explosion occurs, specifically, the effect of experimental parameters in the dispersion. The experimental parameters studied in this paper are temperature and flow regime. In this study, various computational fluid dynamics models were used to simulate the dispersion of the particles. The RSM-w turbulence model produced the most accurate projection of all the models used for turbulent regimes. However, the turbulence model SST k-w is the most steady and secure model. Aside from that, it also requires fewer equations to function, unlike the other models. In the other model, realizable k-e, a continuity error occurred. Thus, a new study development must be conducted to resolve the error. Furthermore, researchers must focus on designing numerical models that give accurate results while staying stable and requiring as simple and minimal calculations as possible.

In the study conducted by Shengbin Di et al. [17]., the researchers put forth an innovative approach to tackle the challenges associated with modeling dynamic fluid-solid interactions. They introduce an improved direct-forcing immersed boundary method that aims to enhance the numerical representation of particle dispersion in such systems. The accurate depiction of fluid-solid interactions is crucial for understanding the behavior and movement of particles in various applications, including environmental processes, industrial systems, and biological systems. Simulating fluid-solid interactions has traditionally been a complex task due to the inherent difficulties in accurately capturing the intricate dynamics. The direct-forcing immersed boundary method offers a promising solution by directly imposing the forces exerted by the fluid on the solid particles. This eliminates the need for explicit boundary conditions and allows a more accurate representation of the fluid's interaction with particles. The proposed method improves upon existing approaches by refining the representation of fluid-solid interactions. It addresses the limitations and shortcomings of previous models, such as incomplete force coupling and numerical instabilities. By incorporating the improved direct-forcing immersed boundary method, the researchers aim to provide more accurate predictions of particle dispersion, including factors like particle trajectories, velocity profiles, and concentration distributions. The significance of this research lies in its potential applications in a wide range of fields. Understanding particle dispersion is crucial for assessing air and water pollution, studying the behavior of granular materials, analyzing fluidized bed reactors, and simulating the movement of biological particles, among other areas. Accurate modeling of fluid-solid interactions can lead to more reliable predictions and insights, which, in turn, can inform decision-making processes and enable better designs for systems and processes involving particle dispersion.

While the study by Shengbin Di et al. [17] presents a valuable advancement in modeling techniques for fluid-solid interactions, there are still avenues for further research. It is essential to evaluate the performance and robustness of the improved direct-forcing immersed boundary method under different flow conditions, particle shapes, and sizes. Additionally, investigations into integrating additional physical phenomena, such as particle aggregation or breakup, could enhance the model's accuracy. Further exploration and refinement of these modeling approaches will contribute to the continued advancement of our understanding of particle dispersion in fluid-solid systems. There is also a need for further evaluation and validation of the proposed improved direct-forcing immersed boundary method for simulating dynamic fluid-solid interactions. Although the study introduces an innovative approach to enhance the numerical representation of particle dispersion, it is essential to assess the method's performance under various flow conditions, particle sizes, and shapes. Conducting thorough investigations and comparisons with experimental data or alternative modeling techniques would help validate the accuracy and reliability of the proposed method. Additionally, exploring the integration of additional physical phenomena, such as particle aggregation or breakup, would further expand the capabilities and applicability of the model. Addressing these research gaps would contribute to advancing and refining modeling techniques for fluid-solid interactions, ultimately improving our understanding of particle dispersion in diverse scenarios.

In the study by R. Huang [18], a particle-filter-based online method for degradation analysis is proposed, explicitly focusing on applying the exponential-dispersion process. The exponential-dispersion process is a versatile stochastic model encompassing various degradation processes, making it suitable for analyzing various systems and phenomena. The fundamental motivation behind the research is to address the challenges posed by continually updating degradation observations and the need for real-time analysis. Traditional offline methods may struggle to handle the continuous influx of new data and require storing and recalling historical observations, which can be computationally intensive and impractical for real-time decision-making. Hence, the study seeks to develop an online method to update parameter estimators and dynamically provide real-time degradation analysis results. The proposed method leverages the particle filter technique, a powerful sequential Monte Carlo method, to perform online inference for degradation analysis. The particle filter method allows for iterative parameter estimation using each new observed data point only once, eliminating the need to store and access historical data. By iteratively updating the parameter estimators, the method can adapt to changing degradation patterns and provide up-to-date insights into the degradation process. The study focuses on the Tweedie exponential-dispersion model, a subclass of the exponential-dispersion process. The Tweedie model is known for its flexibility and ability to capture various degradation phenomena. The proposed online degradation analysis method offers a powerful and versatile tool for real-time monitoring and predicting degradation processes by integrating the Tweedie exponential-dispersion model with the particle filter method. The study conducted simulation studies to evaluate the effectiveness of the proposed method. These simulations demonstrate the method's ability to accurately track and analyze degradation processes in real-time, even in the presence of evolving data. By comparing the results of the proposed method with those of traditional offline methods, the study showcases the advantages of online inference in terms of computational efficiency, real-time capability, and adaptability to changing degradation patterns.

Raeini et al. [19] present a spatially resolved fluid-solid interaction model designed explicitly for dense granular packs and soft-sand materials. The research aims to address the limitations of existing models in accurately capturing the complex behavior of fluid-solid interactions in these types of materials. The research highlights the importance of understanding and accurately representing the behavior of granular packs and soft sand in various engineering and geotechnical applications. The authors emphasize that traditional continuum-based approaches often fail to capture the intricate details of fluid-solid interactions, leading to inaccurate predictions and limiting the applicability of the models. To overcome these limitations, the study proposes a spatially resolved model that considers the individual particles and their interactions within the granular pack or soft-sand system. The model incorporates discrete particle dynamics and explicitly accounts for the fluid flow through the void spaces between the particles. Employing advanced numerical techniques, such as the discrete element method (DEM) and computational fluid dynamics (CFD), the model accurately captures the behavior of individual particles and their interaction with the surrounding fluid. This enables a more realistic representation of fluid-solid interactions in dense granular packs and soft-sand materials. The proposed spatially resolved model offers a more comprehensive and detailed understanding of fluid-solid interactions in these materials, allowing for improved predictions and insights into their behavior. The research contributes to the field by addressing the gap in accurately modeling fluid-solid interactions in dense granular packs and soft sand materials. This study presents a spatially resolved fluid-solid interaction model for dense granular packs and soft-sand materials. By incorporating discrete particle dynamics and considering the individual behavior of particles within the system, the model provides a more realistic representation of fluid-solid interactions. This research contributes to the advancement of modeling techniques for accurately capturing the complex behavior of granular materials. It expands our understanding of fluid-solid interactions in engineering and geotechnical applications.

The article by X. Mei et al. [20] focuses on developing a high-order Markov chain model to predict the dispersion of particles in indoor environments with varying ventilation modes. The researchers aim to address the challenge of understanding and predicting the movement of particles in indoor spaces, which is crucial for assessing indoor air quality and designing effective ventilation strategies. They propose using a high-order Markov chain model that considers the historical states of the ventilation system to predict future particle dispersion. The study considers different ventilation modes, including natural, mechanical, and combination. By analyzing the data obtained from real-world experiments, the researchers constructed a high-order Markov chain model that captures the complex dynamics of particle dispersion under these ventilation modes. The model accounts for factors such as the concentration and size distribution of particles, as well as the characteristics of the ventilation system. Incorporating these variables, the researchers aim to provide a more accurate prediction of indoor particle dispersion compared to existing models. The study results show that the high-order Markov chain model effectively predicts particle dispersion under dynamic ventilation modes. The model's accuracy is evaluated through comparison with experimental data, demonstrating promising performance in capturing the complex dynamics of indoor particle movement. Overall, the research contributes to indoor air quality assessment by providing a predictive model that can assist in designing efficient ventilation strategies and improving indoor environmental conditions. The study may not have fully accounted for the variability and complexity of real-world indoor environments and ventilation systems. Indoor environments can vary significantly in layout, furniture arrangement, occupancy patterns, and building materials, which can impact particle dispersion. Additionally, ventilation systems can have distinctive designs, operation modes, and control strategies. Future research could address these factors to improve the applicability and generalizability of the high-order Markov chain model. The validation of the high-order Markov chain model may have been limited. While the study mentioned the comparison of model predictions with experimental data, the extent and diversity of the validation may not have been comprehensive. It is essential to validate the model against various experimental setups, including indoor environments, ventilation configurations, and particle sources. This would help assess the model's performance under various conditions and provide more confidence in its predictive capabilities.

Another article by A. Nanni et al. compares Puff and Lagrangian particle dispersion models at a complex coastal site. The researchers aim to evaluate and compare the performance of two diverse models used for simulating the dispersion of particles in the atmosphere. Specifically, they examine the puff model and the Lagrangian particle dispersion model. The study site chosen for this comparison is a complex coastal area, which poses unique challenges for dispersion modeling due to the influence of variable wind patterns, complex terrain, and other coastal factors. The study discusses the methodology employed to evaluate the models and compares their performance based on various metrics. The researchers consider factors such as model accuracy, computational efficiency, and the ability to capture the complex dispersion patterns at the coastal site. Comparing the results obtained from both models, the study provides insights into the strengths and limitations of each approach. The research findings contribute to our understanding of how well the Puff and Lagrangian particle dispersion models perform in complex coastal environments and provide guidance for choosing the most suitable model for similar locations. The study compares the performance of the Puff and Lagrangian particle dispersion models at a complex coastal site. The study evaluates model accuracy and computational efficiency, providing insights into the strengths and limitations of each model type in capturing the complex dispersion patterns in coastal environments. Based on the general context of particle dispersion modeling, there is limited consideration of model uncertainties: The study may not have extensively addressed the uncertainties associated with the Puff and Lagrangian particle dispersion models. These models rely on various assumptions and simplifications, which can introduce uncertainties in their predictions. Evaluating and quantifying the uncertainties associated with the models' outputs would provide a more comprehensive understanding of their reliability and help assess their applicability in complex coastal environments [21].

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References

1. M. Peksen, Multiphysics Modelling of Interactions in Systems, in: Multiphysics Modelling, Elsevier, 2018: pp. 139–159. https://doi.org/10.1016/B978-0-12-811824-5.00005-5.
2. J.B. Johnson, An Introduction to Atmospheric Pollutant Dispersion Modelling, in: ECAS 2022, MDPI, Basel Switzerland, 2022: p. 18. https://doi.org/10.3390/ecas2022-12826.
3. J.P.G. Van Leuken, A.N. Swart, A.H. Havelaar, A. Van Pul, W. Van der Hoek, D. Heederik, Atmospheric dispersion modelling of bioaerosols that are pathogenic to humans and livestock – A review to inform risk assessment studies, Microb Risk Anal. 1 (2016) 19–39. https://doi.org/10.1016/j.mran.2015.07.002.
4. R.K. Jain, Z. "Cindy" Cui, J.K. Domen, Environmental Impacts of Mining, in: Environmental Impact of Mining and Mineral Processing, Elsevier, 2016: pp. 53–157. https://doi.org/10.1016/B978-0-12-804040-9.00004-8.
5. A.G. Silveira, C.S. Maués, C.S. Guimarães, A RSTUDIO-based modeling program for dispersion of particulate matter emissions using Gaussian plume equation, J Phys Conf Ser. 1938 (2021) 012013. https://doi.org/10.1088/1742-6596/1938/1/012013.
6. L. Xie, Z.-H. Luo, modeling and simulation of the influences of particle-particle interactions on dense solid–liquid suspensions in stirred vessels, Chem Eng Sci. 176 (2018) 439–453. https://doi.org/10.1016/j.ces.2017.11.017.
7. F. Rousta, B. Lessani, G. Ahmadi, Particle dispersion and deposition in wall-bounded turbulent flow, International Journal of Multi-phase Flow. 158 (2023) 104307. https://doi.org/10.1016/j.ijmultiphaseflow.2022.104307.
8. I. Pisso, E. Sollum, H. Grythe, N.I. Kristiansen, M. Cassiani, S. Eckhardt, D. Arnold, D. Morton, R.L. Thompson, C.D. Groot Zwaaftink, N. Evangeliou, H. Sodemann, L. Haimberger, S. Henne, D. Brunner, J.F. Burkhart, A. Fouilloux, J. Brioude, A. Philipp, P. Seibert, A. Stohl, The Lagrangian particle dispersion model FLEXPART version 10.4, Geosci Model Dev. 12 (2019) 4955–4997. https://doi.org/10.5194/gmd-12-4955-2019.

9. E. Shavrina, V.-T. Nguyen, Z. Yan, B.C. Khoo, Fluid-Solid Interaction Simulation Methodology for Coriolis Flowmeter Operation Analysis, Sensors. 21 (2021) 8105. https://doi.org/10.3390/s21238105.
10. X. Li, F. Wang, D. Zhang, S. Gu, X. Gao, Fluid-solid interaction simulation for particles and walls of arbitrary polygonal shapes with a coupled LBM-IMB-DEM method, Powder Technol. 356 (2019) 177–192. https://doi.org/10.1016/j.powtec.2019.08.006.
11. X. Tang, Y. Yue, S. Wang, Y. Shen, Modelling of gas-solid-liquid flow and particle mixing in a rotary drum, Powder Technol. 409 (2022) 117758. https://doi.org/10.1016/j.powtec.2022.117758.
12. S.M. Oh, C.H. Lee, S.Y. Kim, Processing method determines the long-term stability of particle dispersions in concentrated nanoparticle/polymer suspensions, Soft Matter. 18 (2022) 841–848. https://doi.org/10.1039/D1SM01428E.
13. J. Saxby, F. Beckett, K. Cashman, A. Rust, E. Tennant, The impact of particle shape on fall velocity: Implications for volcanic ash dispersion modelling, Journal of Volcanology and Geothermal Research. 362 (2018) 32–48. https://doi.org/10.1016/j.jvolgeores.2018.08.006.
14. F.M. Beckett, C.S. Witham, M.C. Hort, J.A. Stevenson, C. Bonadonna, S.C. Millington, Sensitivity of dispersion model forecasts of volcanic ash clouds to the physical characteristics of the particles, Journal of Geophysical Research: Atmospheres. 120 (2015) 11,636-11,652. https://doi.org/10.1002/2015JD023609.
15. D.G.F. Huilier, An Overview of the Lagrangian Dispersion Modeling of Heavy Particles in Homogeneous Isotropic Turbulence and Considerations on Related LES Simulations, Fluids. 6 (2021) 145. https://doi.org/10.3390/fluids6040145.
16. R. Eberwein, A. Rogge, F. Behrendt, C. Knaust, Dispersion modeling of LNG-Vapor on land – A CFD-Model evaluation study, J Loss Prev Process Ind. 65 (2020) 104116. https://doi.org/10.1016/j.jlp.2020.104116.
17. S. Di, W. Ge, Simulation of dynamic fluid–solid interactions with an improved direct-forcing immersed boundary method, Particuology. 18 (2015) 22–34. https://doi.org/10.1016/j.partic.2014.05.004.
18. R. Huang, W. Peng, A Particle-Filter-Based Online Method for Degradation Analysis with Exponential-Dispersion Process, in: 2020 Asia-Pacific International Symposium on Advanced Reliability and Maintenance Modeling (APARM), IEEE, 2020: pp. 1–6. https://doi.org/10.1109/APARM49247.2020.9209330.
19. P.A. Gago, A.Q. Raeini, P. King, A spatially resolved fluid-solid interaction model for dense granular packs/soft-sand, Adv Water Resour. 136 (2020) 103454. https://doi.org/10.1016/j.advwatres.2019.103454.
20. X. Mei, C. Zeng, G. Gong, Predicting indoor particle dispersion under dynamic ventilation modes with high-order Markov chain model, Build Simul. 15 (2022) 1243–1258. https://doi.org/10.1007/s12273-021-0855-y.
21. A. Nanni, G. Tinarelli, C. Solisio, C. Pozzi, Comparison between Puff and Lagrangian Particle Dispersion Models at a Complex and Coastal Site, Atmosphere (Basel). 13 (2022) 508. https://doi.org/10.3390/atmos13040508.