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Recent Advances in Modeling of Particle Dispersion †

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Abstract: Recent advancements in particle dispersion modeling have significantly enhanced our understanding and capabilities in predicting and analyzing the behavior of particulate matter in various environments. However, this field still confronts several research gaps and challenges that span across scientific inquiry and technological applications. This paper reviews the current state of particle dispersion modeling, focusing on various models such as Lagrangian, Eulerian, Gaussian, and Box models, each with unique strengths and limitations. It highlights the importance of accurately simulating multi-phase interactions, addressing computational intensity for practical applications, and considering environmental and public health implications. Furthermore, the integration of emerging technologies like machine learning (ML) and artificial intelligence (AI) presents promising avenues for future advancements. These technologies could potentially enhance model accuracy, reduce computational demands, and enable handling complex, multi-variable scenarios. The paper also emphasizes the need for real-time monitoring and predictive capabilities in particle dispersion models, which are crucial for environmental monitoring, industrial safety, and public health preparedness.

Keywords: fluid–solid interaction; particle dispersion; Lagrangian; Eulerian; Gaussian; box model

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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 small they are, we might not be able to look at the materials and see the enormous clusters. We can determine the size of the 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 fields of structural mechanics and fluid dynamics [1]. Several new models, like Computational Fluid Dynamics, have also been developed. Moreover, the accuracy of the data acquired is continuously enhanced by next-generation representations [2].

2. Theoretical Background

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, the Eulerian model, the Gaussian model, and the box model.

2.1. Lagrangian Approach

According to the Lagrangian method, a 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 of time. 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 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, the distribution of particle sizes, and particle density. Despite its dynamic nature, 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 turbulent air movement and diffusion. The left-hand side of the equation represents the 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 denotes the coefficient of diffusion [3].

2.2. Eulerian Approach

In Eulerian analysis, measurements are made at a predetermined fixed location in space, where an observer's concentration at a particular location 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 in a frame that is moving with the average stream, akin to a person moving simultaneously with the particles. Because of this, forward and backward routes can be generated, which can aid in visualizing 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, areas of the land, and heights and depths of the land. These two models have an average of 1 km to 100,000 km of spatial resolution. 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 simulations that would need a scale close to real-life proportions are suitable for Computational Fluid Dynamics (CFD). However, CFD needs an enormous amount of data, unlike other models, to achieve this.

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

Equation (3) has a steady-state assumption. The equation estimates the concentration at any point in the direction of the source from 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: the Gaussian plume and the Gaussian puff models. The Gaussian model that comprises a permanent point is the Gaussian plume. The Gaussian plume model contains the equation encapsulated in the Lagrangian model. The 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 air pollutant particles and the atmosphere's stability. Environmental permitting processes frequently rely on Gaussian plume models, such as the Industrial Source Complex (ISC), the AERMIC Model within the AERMOD software, and CALPUFF, developed by the United States Environmental Protection Agency (US EPA), as well as the Atmospheric Dispersion Modeling System-Urban (ADMS-Urban), developed by Cambridge Environmental Research Consultants (CERC). Thus, although the AERMOD software has superseded the ISC model, the latter is still widely utilized. This can be explained by the lack or inaccessibility of the input data needed by the AERMOD software and other more complex models [5].

Among the inputs are the pollutant release rate, the release height, the wind speed (at the reference height, frequently the height at which emissions are released), the 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].

2.4. Box Model

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

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

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 width of the box; H is the height of the box (mixing height); and u is the wind speed normal to the box.

3. Recent Advances in Modeling Particle Dispersion

Particle dispersion modeling has several 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 conducted in actual conditions. Currently, the standard methods to study the dispersion of particulate matter in turbulent flow are the eddy interaction model, the Monte Carlo method, and random walk models. The methods mentioned 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 the 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 models [5].

One application of atmospheric dispersion modeling is the analysis and assessment of risk. The authors of [6] conducted a study on liquefied natural gas dispersion once an explosion occurs, specifically the effect of experimental parameters on dispersion. The experimental parameters studied in the paper were temperature and flow regimes. In the study, various CFD models were used to simulate the dispersion of particles. The RSM-w turbulence model produced the most accurate projection of all the models used for turbulent regimes. However, the SST k-w turbulence model is the most steady and secure model. Additionally, it also requires fewer equations to function, unlike the other models. In another model, the realizable k-e, a continuity error occurred. Thus, a new study must be conducted to resolve the error. Furthermore, researchers must focus on designing numerical models that give accurate results while remaining stable and requiring as simple and minimal calculations as possible.

In the study conducted by Shengbin Di et al. [7]., 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. [7] 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 [8], 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 demonstrated 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. [9] 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. It 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. The 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 study by X. Mei et al. [10] 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 a combination of them. 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 study 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 [11].

4. Research Gaps and Future Outlook

The field of modeling particle dispersion has witnessed substantial advancements in recent years, but it still confronts a myriad of research gaps and future challenges. These challenges span across the spectrum of scientific inquiry and technological application, reflecting the complexity and significance of particle dispersion in various contexts, from environmental science to public health.

One of the critical areas where current models often fall short is accurately simulating multi-phase interactions. Particles in both natural and artificial environments interact with a variety of phases, such as gases, liquids, and solids. These interactions are inherently complex and have a profound impact on the behavior and eventual fate of the particles. However, current models typically employ simplifications that may not fully capture the intricacies of such interactions, especially in conditions of high particle concentration or in the presence of reactive or hygroscopic particles. Future research needs to focus on developing models that can more precisely mimic these complex interactions, possibly through enhanced understanding of the physicochemical properties of particles and their behavior under varied environmental conditions.

Another significant challenge is the computational intensity of high-fidelity particle dispersion models. These models, while robust and detailed, often demand extensive computational resources, limiting their practicality for large-scale or real-time applications. This is a considerable constraint, particularly in scenarios requiring quick modeling responses, such as in urban pollution analysis or during industrial accidents. The future of particle dispersion modeling lies in striking a balance between accuracy and computational efficiency, possibly through innovative computational methods, optimization algorithms, and leveraging advances in high-performance computing.

The environmental and public health implications of particle dispersion are increasingly coming to the forefront. Models capable of accurately predicting the dispersion of pollutants and their subsequent interactions with the environment are vital for informed environmental policy making and conservation efforts. Similarly, in the realm of public health, models that can effectively simulate the spread of airborne pathogens are crucial for managing and mitigating the impacts of disease outbreaks. Future research in this area would not only need to address the physical and chemical aspects of dispersion but also integrate biological and ecological dimensions.

The incorporation of emerging technologies like machine learning (ML) and artificial intelligence (AI) presents a promising direction for the evolution of particle dispersion models. These technologies hold the potential to significantly enhance the accuracy of models, reduce computational demands, and enable the handling of complex, multi-variable scenarios that traditional models struggle to address. ML and AI can aid in recognizing patterns, predicting complex system behaviors, and managing large datasets, all of which are common challenges in particle dispersion modeling.

The development of models that can provide real-time monitoring and prediction of particle dispersion represents a significant leap forward. Such capabilities are crucial for various applications, including environmental monitoring, industrial safety, and public health preparedness. Achieving this requires advances not only in modeling techniques but also in sensor technology and data processing capabilities.

Climate change poses a new dimension of challenge for particle dispersion models. Future models will need to account for changing climatic conditions and their impacts on particle behavior. This is a relatively unexplored area that is gaining importance as the effects of climate change become more pronounced.

Tackling the challenges in particle dispersion modeling demands an interdisciplinary approach. Collaboration across disciplines such as physics, chemistry, environmental science, computer science, and engineering is essential. The complexity of the problems requires diverse expertise and perspectives to develop more comprehensive and accurate models.

As models become more refined and capable, they will increasingly influence environmental and public health policies. It is crucial for researchers to work closely with policymakers to ensure that the insights gleaned from advanced models are effectively translated into actionable regulations and guidelines.

In summary, while recent advances in particle dispersion modeling have been significant, the field continues to face a multitude of challenges. Addressing these challenges requires a multifaceted approach that encompasses advanced scientific research, computational innovation, and the integration of emerging technologies. The potential impacts of these advancements are vast, ranging from improved environmental protection and industrial safety to enhanced public health response and policy development. By pushing the frontiers of particle dispersion modeling, we can gain a deeper understanding of these complex systems and their implications, paving the way for a healthier and safer environment.

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