

A review of research on vehicle exhaust dispersion model based on CFD simulation technology

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Abstract. CFD, comprising multiple types of softwares, involves complex technological theories and is used to solve profound issues with a huge amount of calculation. Given the complexity and profundity, this study selects Fluent, OpenFOAM and Star-CCM+ as representatives to review the application of the CFD simulation technology in the vehicle exhaust dispersion models. Fluent, a commercial CFD software, started relatively early and has so far been the most widely used in the field of motor vehicle exhaust dispersion research; OpenFOAM, is open source and has a large number of models and algorithms. Apart from supporting pure model research, OpenFOAM has broad application prospects in coupling with the mesoscale model WRF to improve the accuracy of pollutant dispersion simulation; Star-CCM+, less applied in the research field of vehicle exhaust dispersion, focuses more on vehicle air conditioning system, vehicle radiator, refueling, vehicle aerodynamic noise source simulation and other related fields. The research provides theoretical basis and scientific reference for the application of CFD in the field of urban block-scale air quality research. In the future, with the rapid development of computer technology and the introduction of new theories and intelligent algorithms, CFD technology is very likely to achieve new breakthroughs and continue to enjoy even wider application in the research of motor vehicle exhaust dispersion.

1 Introduction

With the growing ownership of motor vehicles in China, motor vehicle pollution has become increasingly severe, and has contributed as an important source to urban and regional air pollution. Statistics show that pollutants from mobile sources account for more than 30% of nitrogen oxide (NO_x) emissions countrywide. The impact of traffic pollutants

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has been increasingly felt in key areas such as Beijing-Tianjin-Hebei, Fenwei Plain, Yangtze River Delta, Chengdu and Chongqing. Mobile emissions have become the primary source of fine particulate matter (PM_{2.5}) in some cities. As a type of near-ground emissions, motor vehicle exhaust is hard to disperse in urban areas with a high density of both traffic network and population, and a large amount of traffic. The closely packed buildings are not conducive to the dispersion of pollutants either. The pollutants from motor vehicles are especially harmful to citizens long exposed to the traffic environment or living in areas with high traffic density.

To give a quantitative evaluation of the environmental impact of motor vehicle exhaust in a more accurate way, CFD simulation technology has been widely used in the study of vehicle exhaust dispersion. CFD simulation technology is a numerical simulation of convective motion governed by basic flow equations (mass conservation equation, momentum conservation equation, energy conservation equation). Its spatial resolution is up to the meter level, and basic physical quantities (speed, pressure, temperature, concentration, etc.) at each position of the flow field of extremely complex problems can be obtained, so that the turbulence characteristics, spatial distribution, etc. can be determined given the changes of these physical quantities over time^[1-2].

However, since CFD, comprising a wide array of software, involves complex technological theory and is used to solve profound issues with a huge amount of calculation, the application of CFD on actual roads in typical cities is not that widespread. This paper thus reviews the studies the current model research and explores the application status of CFD simulation technology in vehicle exhaust dispersion, with an aim of providing theoretical basis and scientific reference for the application of CFD in the field of urban block-level air quality research.

2 A brief introduction to CFD simulation technology

CFD simulation technology employs computer digital methods to describe motions such as fluid flow and heat transfer. It has the ability to use flexible small grids to deal with complex canyon walls and other boundary conditions. Equipped with advanced turbulence treatment schemes, it is suitable for simulating the dispersion of small-scale pollutants^[3]. CFD is the product of modern fluid mechanics, numerical mathematics and computer science combined. The rapid progress of computer science provides a basic guarantee for the development of CFD, which in turn makes the numerical simulation of pollutant transmission and diffusion more accurate. Therefore, CFD enjoys broad prospects in the field of air quality prediction with its powerful numerical simulating and modeling capabilities.

CFD software generally consists of three parts: pre-processing, solver, and post-processing. The main function of pre-processing is to create geometric models and divide the mesh. The solver is mainly used to determine the control equations of the CFD method, select the appropriate discrete method, choose the numerical calculation method and input related parameters. The post-processing is mainly for the visualization of data, such as velocity field, temperature field, pressure field and other parameters.

Common CFD software includes Fluent, OpenFOAM, Star-CCM+, Star-CD, Flow-3D, CFX, Comsol, Phoenics, etc. This study reviews the three mostly used CFD software in vehicle exhaust dispersion, namely Fluent, OpenFOAM, Star-CCM+, with a focus on their characteristics and the progress of the research on their application.

3 Application of CFD simulation technology

3.1 Fluent

Fluent is currently one of the most popular commercial CFD software packages at home and abroad used to simulate and analyze fluid flow in complex geometric areas. It has a wealth of physical models, advanced numerical methods, and powerful pre- and post-processing functions. Fluent has the advantages of accuracy, adaptability and potential for further development for the simulation of actual road scenarios. In recent years, it has been increasingly applied in the research of motor vehicle exhaust dispersion.

The main features of Fluent include: 1) It has a diversity of grid types including two-dimensional, three-dimensional and hybrid grids; 2) Both Steady and unsteady flow simulations can be performed; 3) It is the commercial CFD software with the most algorithms: non-coupling implicit algorithm, coupling explicit algorithm, and coupling implicit algorithm; 4) It can realize the calculation of both Newtonian fluid and non-Newtonian fluid; 5) It is equipped with a user-friendly interface; 6) It has a powerful parallel computing function [4].

The application of Fluent in the research of motor vehicle exhaust dispersion started early in countries outside China. Murena et al. [5] used Fluent to simulate urban street canyons with different height-width ratios and found that it could simulate various types of roads with strong adaptability. Chang et al. [6] compared Fluent's simulation with wind tunnel experiment and found that the results of the Fluent's simulation agreed with the observation results of the wind field and pollutant concentration field in the street canyon simulated by the wind tunnel experiment. Based on the above research conclusions, many foreign scholars have continued to use Fluent to simulate the dispersion of exhaust in street canyons. Yassina et al. [7] used Fluent's simulation to analyze the impact of road intersections in urban canyons on the flow of motor vehicle exhaust and gas pollutants; Wen and Malki-Epshtein [8] used Fluent to study the influence of roof height and shape on air pollution dispersion in street canyons; Ming et al. [9] studied the law of pollutant diffusion in street canyons and the mechanism of multi-field coordination also using Fluent as the tool.

Domestic scholars started to use Fluent to study atmospheric environmental problems on block scale from as early as 2000 and have achieved rapid progress ever since. Li Lei et al. [10] used Fluent to establish a three-dimensional street intersection model. The simulation shows that Fluent can generate reasonable results of the built model and have broad prospects in the future study of atmospheric environment problems on block scale. Zhang Zhao et al. [11] used Fluent to establish a three-dimensional street model consisting of three streets and two intersections; and simulated the distribution of the wind field and concentration field under two wind directions and two wind speeds. The simulation results show that Fluent can simulate the impact of complex layout of buildings on the atmospheric environment and deliver logical outcomes. Fluent is proved to have good application prospects in issues related to the atmospheric environment of the street and block. Since then, various scholars [12-13] have applied Fluent to study the dispersion of pollutants in different lanes in urban street canyons and explored the characteristics and contributing factors of the evolution and diffusion of vehicle emissions.

The above-mentioned research mostly focused on the static physical factors in street canyons, while in real world scenario, the wind speed and direction of the urban boundary layer as well as the number of cars are constantly changing. Given the fact that the impact of dynamic changing factors on the internal flow of the street canyon is less studied, Wang

Le et al. ^[14] based their research on actual measurement data, adopted dynamic velocity inlet boundary conditions and dynamic pollutant source terms, and improved the wind field and pollutant dispersion in the street canyon under the dynamic boundary or source term simulated by the mathematical model of Fluent. The results show that the distribution and peak of pollutant concentration in a dynamic environment are jointly determined by the wind field and changes of traffic flow. The simulation provides the wind speed and traffic flow data which are changing and have real time effect without considering the influence of the time and place of the observation. Wang Jiwu et al. ^[15] selected Zhongshan Road, Hangzhou, which has significant morphological characters of street canyons, and used Fluent to conduct numerical simulation experiments on airflow field and carried out research on the space morphology of the street canyon, before drawing out the shape of the street canyon and the basic law of pollutant dispersion. Further plans and designing strategies on how to promote air circulation as well as pollutant dispersion and dilution have been proposed based on the research findings.

Faced with the problem that the existing research on the architectural layout of street canyons mainly focuses on a single source of pollution and ignores the impact of the street side, Zhan Naiyan et al. ^[16] used the numerical simulations of Fluent to analyze the airflow field and the law of pollutant concentration dispersion in the micro-environment of the block, targeting on the street canyons under three typical architectural layouts in urban blocks. The experiment includes both the comparison of the differences under different building layouts, but also the horizontal comparison of the two street canyons from the same layout, thus providing theoretical basis for the effective dispersion of the pollutants and the job of future planning from the urban construction department.

Yu Haijun et al. ^[17] coupled Fluent with the mesoscale weather software WRF and the region-scale air quality model CMAQ, and adjusted the simulation accuracy to 1-10 m. The simulation results were compared with the monitoring data, and the results proved the feasibility and even higher accuracy of the coupling. This is the preliminary application of Fluent coupled with the mesoscale model WRF and CMAQ in the study of air pollution in small areas of the underlying surface of the city. It provides a scientific methodological basis for obtaining more accurate and precise environmental data of urban pollutants.

3.2 OpenFOAM

OpenFOAM is an open source program package for solving continuity equations based on the finite volume method. It is mainly used to solve fluid flow and heat transfer problems. As a piece of open source CFD software, it is essentially a pre-compiled function library. There are currently more than one million lines of code and dozens of models. Users can either directly use simple commands to solve simple problems, or modify and integrate these function libraries when the need arises, so as to develop the CFD software as needed to adapt to changing problems ^[18].

The structure of OpenFOAM is shown in Figure 3.2-1. It can be traced back to the research of the David Gosman's team in Imperial College London in the 1980s and was released as a piece of open source software in 2004. It can be used and distributed freely, thus has been welcomed by the majority of researchers. At the same time, the contributions of the open source software community have also enriched OpenFOAM's models and algorithms. Up till now, multiple branches that can perform simulation in different fields have been derived from OpenFOAM, extending its function to areas such as pollutant dispersion, fluid-solid coupling, and multiphase flow ^[19].

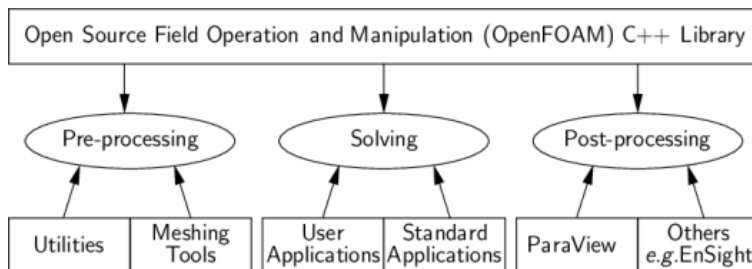


Fig. 1. OpenFOAM structure.

OpenFOAM has the following advantages: 1) OpenFOAM is completely open source, there is no license fee, and researchers can use it for free. The results of secondary development can be freely disseminated in the academia; 2) The programming language is object-based, with easy-to-read syntax for equation solving, and detailed code introduction is provided officially, which is very friendly to secondary development; 3) The unstructured polyhedral grids based on the finite volume method can help with the capture of complex shapes; 4) Most applications in OpenFOAM can be operated in parallel with a fast running speed, which is suitable for large-scale calculations on supercomputers; 5) It has a huge application and model library. As mentioned above, there are already a large number of models and algorithms in OpenFOAM, and they can be directly used to solve practical problems. Even if the existing models and algorithms cannot address the current problems, an application that meet the actual needs can be developed based on the preliminary version with only a small amount of secondary work.

Given the above-mentioned advantages, OpenFOAM has been chosen by many scholars at home and abroad to conduct research on pollutant dispersion. Chen Cunyang et al. [20] used the Yishan campus of Fuzhou University as the virtual geographic environment of the dispersion zone, and used OpenFOAM to simulate the dispersion process of chlorine—the hypothetical poisonous gas. Through comparing the simulation results of ρ (Cl_2) in Fluent under the same conditions, it has been found that OpenFOAM, combined with the PISO algorithm, can well perform the simulation of the toxic gas dispersion process in a complex virtual geographic environment. Compared with Fluent, OpenFOAM enjoys an average deviation which is less than 5%, but an improved calculation efficiency by 41.89%. At the same time, the research shows that the numerical simulation based on the PISO algorithm has the advantages of strong tolerance and relatively stable calculation in large-scale toxic gas dispersion simulations such as in the scenario of urban blocks. Jeanjean AP R et al. [21] used OpenFOAM's $k-\epsilon$ turbulence model to study the combined effects of building morphology and trees on the concentration of air pollutants in the Marylebone community in central London, with the influence of trees addressed through porous media. The study found that in order to achieve a comprehensive assessment and help urban planners with their sustainable design of the plantation of trees in the urban environment, it is necessary to consider the aerodynamics of trees and the dispersion effects in the CFD model. Buccolieri R et al. [22] used OpenFOAM's steady-state simulation to evaluate the effects of trees with different leaf area densities on ventilation, nitrogen oxides and $\text{PM}_{2.5}$ concentrations at different heights in the street canyon of Marylebone Rd, London. The results show that planting trees is beneficial to street areas both close to and far away from the trees. Influenced by the aerodynamics, the average concentration of pedestrians is reduced by 18%. Chatzimichailidis A E et al. [23] used a typical quasi 2D street canyon geometric model and OpenFOAM to study and verify the main parameters that affect the LES transient simulation of pollutant dispersion. A LES parameter

configuration that is easy to reuse has been proposed, which provides a satisfactory compromise between calculation requirements and accuracy.

In addition to conduct research purely based on CFD models, some researchers have proposed that the coupling of CFD and WRF can improve the accuracy of pollutant dispersion simulation. Tewari M et al. [24] evaluated the impact of the coupling of a micro-scale CFD model and a mesoscale NWP (numerical weather prediction) model on the accuracy of the modeling of pollutant dispersion in urban areas. It is found that when the wind field generated by the downscaled WRF is used as the initial and boundary condition, the predictive ability of the CFD model has been significantly improved. A key reason is that the turning of the lower boundary-layer wind and pressure gradient is well reflected in the transient three-dimensional WRF field. Consequently, many scholars have started to look into the the boundary conditions given by the mesoscale model when it is coupled with a CFD model. The coupling of WRF and CFD also has been used by Zheng Yijia et al. [25] to study the structure of the atmospheric boundary layer, crosswind, location of pollution sources and their influence on the wind flow field and pollutant distribution in the urban built-up areas (UBA) of Shenyang, China. It is found that the atmospheric boundary structure plays a vital role in the pollution inside the building complex. It determines the potential turbulent dispersion capacity of the surface of the atmosphere; the change of the crosswind direction can significantly affect the dispersion pattern of pollutants, which is a more sensitive factor than the crosswind speed; Under a given atmospheric state, the location of the pollution source will to a large degree affect the pollution pattern in the UBA. At the same time, the study points out that WRF-CFD numerical evaluation is a reliable method to evaluate the complex flow and dispersion in UBA.

At present, one of the most widely used CFD software pieces for WRF-CFD coupling research on the dispersion of pollutants is OpenFOAM. Miao Y et al. [26] conducted a numerical study on the diffusion of airflow and pollutants in a complex urban area in Beijing through the coupling of OpenFOAM and mesoscale weather models. To start with, the simulation accuracy of OpenFOAM was verified through comparison with the wind tunnel experimental data. The results of the coupled model simulation show that the airflow around the actual building is very different from the ambient wind on the boundary provided by the WRF model. Under the influence of the building, the pollutant dispersion model is highly complicated. Near ground pollutant were highly concentrated in both the descending and ascending slots, but the reasons for this high concentration level in each configuration are different: in the former case, it is caused by the weaker vertical flow; while in the latter case, it is caused by a downward moving vortex. The results of this study show that the WRF-OpenFOAM coupling model is an important tool that can be used to study and predict urban flow and diffusion in densely built-up areas. Liu Y et al. [27] proposed a multi-scale modeling method that combines the WRF (weather research and forecasting) model with the open source CFD simulation tool OpenFOAM. This coupling method can simulate the wind current and pollutant distribution in UBA with high-resolution grids, in which the mesoscale model WRF provides boundary conditions for the microscale CFD model OpenFOAM. The advantage is that the actual weather conditions are considered in the CFD simulation, and through the meshing function of OpenFOAM, complex building layouts can be easily handled. The joint urban tracer diffusion experiment conducted in Oklahoma City in 2003 also shows an excellent agreement between CFD simulation and field observation.

3.3 Star-CCM+

As a piece of CFD commercial software, Star-CCM+, combining continuum mechanics numerical technology and software engineering technology while equipped with excellent design, can be used to solve comprehensive interdisciplinary problems. It provides the most comprehensive engineering physics simulation in the world, and is mainly used in areas such as fluid or solid flow, heat transfer and stress.

Compared with general CFD software, Star-CCM+ is more efficient and convenient in that it does not require separate post-processing, for it could perform result processing all by itself. At the same time, Star-CCM+ also has these following merits: 1) Simulations are based on multiphysics and continuous medium; 2) Physical model and grid size can be set separately; 3) It has the generalized interface; 4) It is equipped with surface-based solver which supports many different types of grids; 5) It could exercise dynamic control of the simulation process [28].

Li Qing et al. used the numerical simulation of Star-CCM+ to study the dispersion of carbon monoxide, hydrocarbons, nitrogen oxides, and particulate matter in the atmosphere. The results show that the simulated values are in good agreement with the measured values. When the crosswind speed is low, the speed of motor vehicle exhaust dominates the airflow structure and the dispersion of pollutants. When the crosswind speed is greater than that of the motor vehicle exhaust, the vortex and turbulence generated by the interaction of the vehicle exhaust plume and the crosswind can accelerate the dispersion of pollutants [29].

Tan Libin et al. [30] used the fluid analysis software Star-CCM+ to numerically simulate the internal flow field of the air-conditioning system in defrosting, defogging and surface blowing mode, and analyzed whether the air volume distribution of each air duct is appropriate, whether the speed distribution of the front windshield is balanced, and how the flow field of the vehicle's air-conditioning system in different working modes is distributed. Tan Libin et al. [31] took the radiators from some low-speed electric vehicle as the research object, applied Star-CCM+ to compare the flow field of the two radiators equipped to serve the whole vehicle, and analyzed the flow field distribution under both idle and maximum speed. The research thus provides a scientific basis for the selection of radiator for the whole vehicle.

Based on the VOF multiphase flow model and turbulence model theory, Zhu Fawang et al. [32] used STAR-CCM+ to numerically simulate the refueling process of the fuel system of a certain vehicle, checked the fuel distribution of the monitoring surface and of the fuel system at different stages, analysed the refueling performance, and compared the results with the actual refueling experiment. It shows that the simulation results are consistent with the actual experiment, which can provide theoretical guidance for pipeline design in the early stage and save the cost of product development. Liu Yang et al. [33] compared the accuracy of Fluent and Star-CCM+ in calculating the sources of vehicle's aerodynamic noise. They carried out a wind tunnel experiment of aerodynamic noise of a hatchback car and performed numerical simulation, and found that the distribution cloud maps of the overall sound pressure level obtained by two software are similar, the characteristics of noise distribution are consistent in each component, and order of the size is the same. Yet Fluent is better than Star-CCM+ in calculating the overall sound pressure level and sound pressure level spectrum of the measuring point.

4 Conclusion and perspectives

To provide theoretical basis and scientific reference for the application of CFD in the field of urban block-scale air quality research, this study selects Fluent, OpenFOAM, and

Star-CCM+ as typical software to review the application of CFD simulation technology in the motor vehicle exhaust dispersion model. The main conclusions are as follows:

(1) Fluent is a piece of commercial CFD software that started relatively early and has so far been the most widely used in the field of motor vehicle exhaust dispersion research. During the application process, some scholars have improved the software according to actual needs. Some scholars have coupled Fluent with the mesoscale models WRF and CMAQ and conducted preliminary applications in the study of air pollution in small areas on the underlying surface of cities, proving this method to be feasible and more accurate.

Research carried out using Fluent as a tool on the dispersion characteristics of exhaust in street canyons are wide reaching, including not only the pattern of pollutant dispersion in different lanes, the distribution of concentration field under different weather conditions, but also the impact that the road intersections, heights and shapes of roofs, and building layouts can have on the dispersion of the exhaust. Studies of the characteristics and influencing factors of the evolution and dispersion of motor vehicle emissions in street canyons with Fluent as a tool provide effective references for environmental protection, urban planning, and motor vehicle production, etc.

(2) OpenFOAM, as a piece of open source CFD software, has a large number of models and algorithms, which can be directly used to solve practical problems, and can also be further developed into applications that meet actual needs. It has been widely applied in the research on the diffusion of pollutants, and has gradually made its way into the dispersion of motor vehicle exhaust as well. As it is open source, OpenFOAM enjoys great prospects when it is coupled with the mesoscale model WRF to improve the accuracy of pollutant dispersion simulation.

The WRF-OpenFOAM coupling model is an important tool for studying and predicting the flow and dispersion of pollutants in urban areas with closely packed buildings. It provides city planners with a reliable environmental modeling tool in UBA, and can be further expanded to include future weather scenario to study of the impact of climate change.

(3) The more mainstream commercial CFD software Star-CCM+ has less application in the research field of vehicle exhaust dispersion. Instead, it is mainly used in the fields of vehicle AC system, vehicle radiator, refueling, vehicle aerodynamic noise source simulation, etc. It aims to provide simulation data support and theoretical reference for the model design of motor vehicles.

The emergence of CFD simulation technology enables scholars to focus on local areas of the city and study micro-scale air pollution problems. It also provides a scientific method for analyzing the pattern of the spread and dispersion of vehicle exhaust around buildings and blocks. OpenFOAM, as a piece of open source software, can obtain a more subtle and accurate wind field and turbulence structure in the canopy when coupled with a mesoscale numerical model, thus providing a broader application prospect in the research of the dispersion of vehicle exhaust pollution.

To conclude, with the rapid development of computer technology, as well as the introduction of new theories and intelligent algorithms in the future, CFD technology is very likely to achieve new breakthroughs and enjoy a wider acceptance in the research field of motor vehicle exhaust dispersion.

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