CFD simulation of chemical gas dispersion under atmospheric boundary conditions

†*George XU[1], Arthur LIM[1], Harish GOPALAN[1], Jing LOU[1] and Hee Joo POH[1]

[1]Fluid Dynamics Department, Institute of High Performance Computing, A*STAR, Singapore.

*Presenting author: xu_xiangguo@ihpc.a-star.edu.sg
†Corresponding author: xu_xiangguo@ihpc.a-star.edu.sg

Abstract

Pollutant control is one of the key concerns in the design of buildings, for the sake of occupational health, safety and environment sustainability. In particular, risk analyses related to emergency leakage of chemicals from storage tanks or chemical processes have aroused increasing attentions in recent days, as well as the effectiveness of mitigation measures in order to eliminate, reduce and control the risks. In this paper, a CFD methodology with non-reactive chemical gases treated as passive scalars has been developed to simulate the gas dispersion across urban environments, subject to atmospheric wind conditions. Special treatments to maintain the consistency in atmospheric flow profiles, turbulence modeling and boundary conditions have also been accounted for. The developed model for gas dispersion has been implemented in the open source CFD code - OpenFOAM. The proposed methodology has been validated by modeling the gas dispersions for two urban-related test cases: the street canyon measured in a laboratory wind tunnel and the Mock Urban Setup Test (MUST) field experiment conducted in the desert area of Utah State. Effects of turbulent Schmidt number have been primarily addressed in this study. Statistical analyses about the discrepancies between predicted and experimental data have been carried out to quantity the accuracy of the proposed methodology. Simulations results from passive scalar transport equation demonstrate good agreement with experimental data, though tracer gases heavier than the atmospheric air were used in the both measurements. Furthermore, sensitivity tests also indicate that the accuracy of the simulation results is sensitive to the value of turbulent Schmidt number.

Keywords: **CFD, gas dispersion, OpenFOAM, urban environment modeling**

Introduction

In the design of residential, commercial, industrial or infra-structure buildings, pollutant control has become an important design feature to be addressed for the sake of occupational health, safety and environmental sustainability. The same concern has been extended for chemical plant design where emergency leakage of chemicals from storage tanks or chemical processes may take place. Risk analysis related to such emergency cases should be carefully investigated during the planning and design stages, and then effective mitigation measures should be proposed and evaluated to eliminate, reduce and control the risks. All these concerns are related to modeling of the gas dispersions.

Chemical gas dispersion in space is conventionally evaluated using empirical methods, such as Gaussian plume modeling [1]. Such empirical methods are very efficient, usually with the consideration of dynamic changes in atmospheric wind conditions. They have been widely adopted to study the impacts of plumes out of chimneys or vent shafts upon the environment within a large space. However, the obstructions due to buildings is one of the drawbacks, in particular near the ground area, cannot be accurately resolved with these methods. Recently, due to the rapid advance in computers, computational fluid dynamics (CFD) method has

become more attractive in assessing the environmental pollution, because its higher accuracy and richer field information. Comparatively, CFD method can be used to accurately predict the pollutant dispersion due to the obstructions of buildings, thus it is more suitable tool to simulate the pollutant dispersion in an urban environment that is highly occupied by high-density of buildings.
Multi-species modeling and passive scalar modeling are the two CFD methods that are usually adopted to simulate gas dispersions. The former can result in high-accuracy prediction, due to the well consideration of most physics relevant. However, it depends on the accuracy and full set of thermodynamic properties of chemical species. Besides, it is very time consuming in simulation. Comparatively, the passive scalar modeling is much more cost effective and less demand in input parameters, which is suitable for quick solutions for engineering problems.

As a part of the objectives for a government-funded project, a passive scalar modeling methodology for non-reactive chemical gases dispersion across urban environments has been developed, subject to atmospheric boundary conditions. The main objective in this study is to characterize the accuracy of passive scalar modeling methodology, when it is applied to simulate chemical gases dispersed in urban environments. Research efforts are limited to the development of efficient solver for dilute dispersion of chemical gases in spaces relatively away from the leakage site. In the proposed methodology, the leaked gas is represented by well-mixed volumetric clouds and the transport equation for passive scalar is adopted to trace the concentration of chemical gases. Special treatments to maintain the consistency in atmospheric flow profiles, turbulence modeling and boundary conditions have also been accounted for. All the development work has been implemented in OpenFOAM [2] – an open source CFD code.

In this paper, the proposed CFD methodology is to be first introduced briefly, followed by the in-depth discussion about the simulation results for two testing cases. Some remarks upon the proposed CFD methodology for gas dispersion modeling are finally summarized in the conclusion section.

CFD Methodology

In this study, steady-state incompressible flows under isothermal conditions are primarily focused. In addition to the continuity and momentum equations, the passive scalar transport equation has been chosen to model the concentration changes. The two-equation k-ε models are adopted to address the turbulence effects.
The governing equation for passive scalar transportation takes the following form:

$$\frac{\partial}{\partial t}(c) + \nabla \cdot (c\mathbf{u}) = \nabla \cdot [(D_c + \nu_t / Sc_t)\nabla c] + S_c \quad (1)$$

where c, $\mathbf{u}$ and t denote the concentration of pollutant, air velocity and time, respectively; D_c and ν_t represent the molecular diffusivity of pollutant of concern and the turbulence kinematic viscosity; S_c is the source term; and Sc_t denote the turbulence Schmidt number.

In the proposed method, the chemical gas released from leakage region is modeled with the source term, S_c. Linearization of the source term, as proposed by Patankar [3] has been adopted during the solution procedure for the sake of improved numerical stability.
Second-order discretization schemes have been adopted to approximate the partial differential terms in governing equations. The resultant algebraic equations are solved with the well-known SIMPLE solution procedure.

Results and Discussion

The accuracy of the proposed methodology has been demonstrated with the solutions to two test cases: gas dispersions across street canyon in a laboratory scale and gas dispersion around a mock up setting test (MUST) under a realistic atmospheric scale. Details about the flow behaviors will be discussed in the following section.

Test Case 1: Street Canyon

The first test case is based on the wind tunnel test for a street canyon configuration that was designed and measured by the Laboratory of Building and Environmental Aerodynamics at the Institute for Hydromechanics (IfH) in the University of Karlsruhe, Germany [4]. As shown in Figure 1, the computational domain consists of two parallel buildings which form the street canyon of concern. Four sub cell zones on the street are chosen to represent the line sources for tracer gas (SF_6), emulating the chemicals emitted from traffic vehicles. The total release rate is 10g/s. Compliant with the test conditions, the power-law wind profile is adopted to represent the incoming wind perpendicular to the street.

Consistent with the measured data, the normalized concentration of tracer gas is calculated as

$$c^{+} = \frac{cu_H H}{Q / l} \tag{2}$$

where u_H is the reference velocity at the building height, H; Q and l denote the gas release rate and the length of the line sources, respectively. It should be noted that the values of c^{+} measured on the leeward and windward surfaces are available for validation.

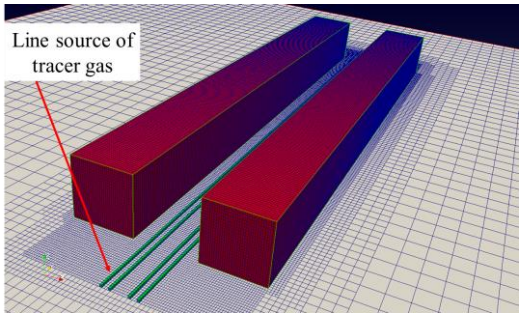


Figure 1. Computational domain and grid.

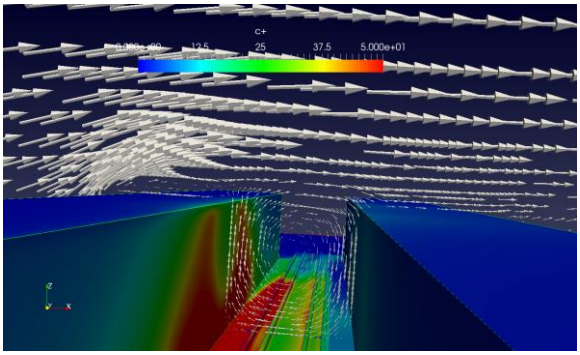
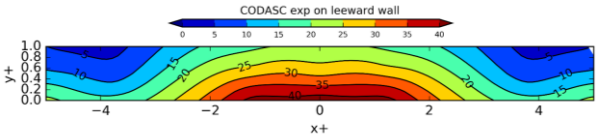


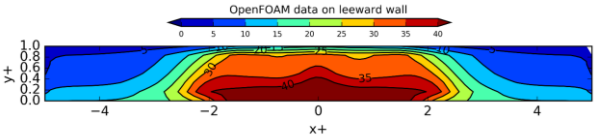
Figure 2. Airflow across the street canyon and contours of gas concentration on wall surfaces.

As shown in Figure 2, the incoming atmospheric wind, perpendicular to the street canyon, induces the recirculated air flow across the canyon, similar to the lid-driven cavity flow. The pollutant released from the sources on the ground turns to follow the airflow travel in space. The downward movement of the airflow along the windward surface turns to clear the pollutant from the respective surface. On the other hand, the recirculated air eventually carry the pollutant to travel towards the opposite building. It results in the higher concentration of the pollutant gas on the leeward surface.

The predicted gas concentration on the leeward and windward surfaces are presented in Figures 3 and 4, where the measured values are also included for comparison. It is apparent that good agreement between the numerical results and the measured values is achieved.

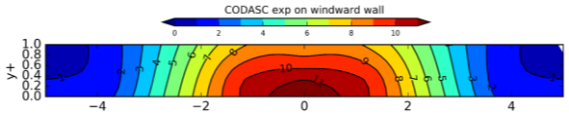


(a) Measurement

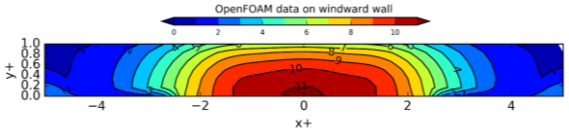


(b) CFD

Figure 3. Contours of c+ on the leeward surface of the street canyon.



(a) Measurement



(b) CFD

Figure 4. Contours of c+ on the windward surface of the street canyon.

Sensitivity studies about different forms of k-ε models, i.e. standard, realizable and RNG k-ε models, have been investigated for the street canyon test case. It is found that standard k-ε model yields the most accurate prediction. Besides, subject to the standard k-ε turbulence model, additional studies about the impact of Sc_t value have also been performed.

Statistical analyses [5] about the predicted and measured values of c^+ on the two building surfaces of concern have been conducted. Fractional Bias (FB), Normalized Mean Square Error (NMSE) and Fraction of Predictions within a factor of two of the observations (FAC2) are selected to quantify the accuracy of the proposed CFD model. As summarized in Table 1, all the values for Sc_t that have been tested produce reasonable results. In addition, the most agreeable prediction with the measurement can be obtained when Sc_t = 0.3.

Table 1. Impacts of Sc_t on the gas dispersion.

Name	Definition	Model Perfects	Acceptable Model	Sc_t		
				0.7	**0.3**	**0.2**
FB	$2\times(\bar{C}_0-\bar{C}_p)/(\bar{C}_0+\bar{C}_p)$	0	-0.3<FB<0.3	-0.39	-0.02	0.17
NMSE	$\overline{(C_0-C_p)^2}/(\bar{C}_0\times\bar{C}_p)$	0	NMSE<4	0.06	0.09	0.11
FAC2	$\bar{C}_0/\bar{C}_p$	1	FAC2>0.5	1.49	1.02	0.84

Test Case 2: MUST

The second case that has been simulated correspond to the airflow across the array of containers geometry of the Mock Urban Setting Test (MUST) field experiment. In the field test, 12 by 10 array of containers (each 12.2m long, 2.42m wide and 2.54m high) were deployed in desert of western Utah to mimic the urban environment. Details about the experimental studies are clearly addressed in DPG Document No. WDTC-FR-01-121 [6].

Test Scenario #2681829, as studied by Bekka *et. al.* [7], is chosen to be simulated with the proposed methodology. In the MUST field test, Propylene (CH_2CHCH_3) was used as tracer gas and released at different locations of concern. In the test scenario simulated here, the release rate of propylene is 225 l/min. Concentration of the released gas at 48 locations, as indicated by elliptic dots in Figure 5, are monitored and compared with the measured values. It should be noted that 40 receptors are located at 1.8m height and additional eight receptors are installed at various vertical heights on the tower located at the centre of the test field.

The neutral-state log-law wind and turbulence profiles, consistent with the atmospheric boundary conditions during the measurement, are implemented as the inflow conditions. To maintain the horizontal homogeneity, as recommended by Blocken [8], changes have been

made to the constants for k-ε turbulence model and wall functions and care has been taken in the grid generation in particular for the first-layer of grid on the ground. A total of 9.6-million hexa-dominated elements have been generated and used in simulations.

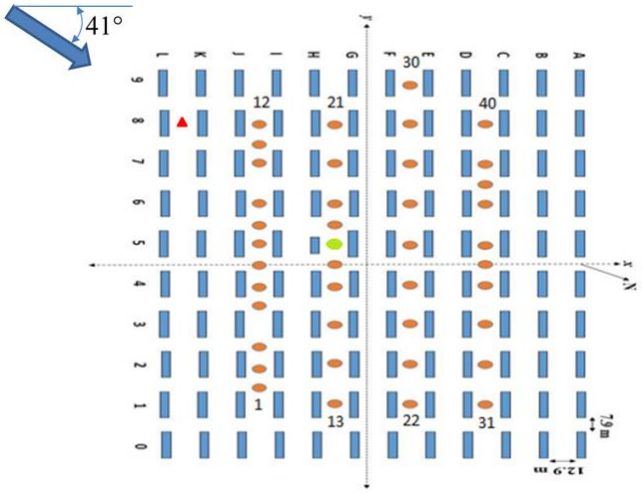


Figure 5. MUST site and locations of receptors for Test Scenario #2681829.
(Courtesy to Bekka *et. al.* [7] for the reuse of their image**).**

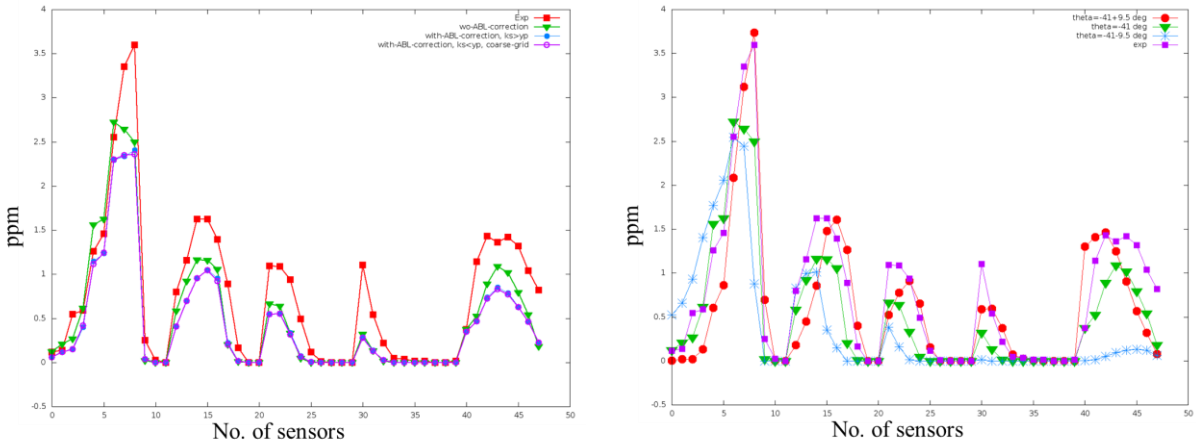
Sensitivity tests about the impacts of Sc_t have been carried out. As summarized in Table 2, predicted results show poor agreement with measured data when Sc_t takes the smaller value, and the most accurate prediction can be achieved when Sc_t becomes as high as 0.9. Thus most of simulations subsequently conducted are based on $Sc_t = 0.9$.

Table 2. Impacts of Sc_t on the gas dispersion.

Name	***Definition***	***Model Perfects***	***Acceptable Model***	***Sc_t***		
				0.3	**0.7**	**0.9**
FB	$2\times(\bar{C}_0-\bar{C}_p)/(\bar{C}_0+\bar{C}_p)$	0	-0.3<FB<0.3	0.60	0.23	0.15
NMSE	$\overline{(C_0-C_p)^2}/(\bar{C}_0\times\bar{C}_p)$	0	NMSE<4	0.87	0.60	0.73
FAC2	$\bar{C}_0/\bar{C}_p$	1	FAC2>0.5	1.85	1.26	1.16

It is interesting to find that the without atmospheric boundary layer (ABL) correction as proposed by Blocken *et. al.* [5], predicted gas concentration show better agreement with experimental results, as shown in Figure 6(a). Besides, the simulated results, subject to ABL correction, seem insensitive to the relationship between sand grain roughness and the height of first-layer ground elements. All these findings are not consistent with the ABL treatment techniques [8]. Details for the reasons behind will be further investigated in future.

Sensitivity studies about the variation in wind direction for the test scenario have been conducted. As indicated in the measurement report [6], for the test scenario of concern here, the change in wind direction is ±9.5°. Two additional simulations have been carried out according to the two extreme wind directions. As shown in Figure 6 (b), it is manifest that the predicted concentrations are sensitive to the change in the wind direction. Better agreement with measured data can be obtained when θ = (-41+9.5)°. Such sensitivity studies demonstrate the complexity in the uncertainties qualification of prediction models, when the real-life measurement data are used for validation.



(a) Effect of ABL correction (b) Effect of wind direction

Figure 6. Comparison of predicted gas concentration with measured at various locations.

Conclusions

A CFD approach for gas dispersion modeling in urban-alike environment has been proposed, subject to atmospheric boundary layer conditions. The chemical gas is represented by passive scalar and the impact of the species transport upon the airflow is neglected.

Numerical tests for two different scales of urban-alike test cases show that the simulation results are agreeable well with the measured data, though tracer gases heavier than air were used in measurement. Sensitivity tests about Sc_t yield different optimal values for the two test cases. This implies that care should be taken in the choice of Sc_t value when Reynolds-averaged turbulence models are adopted to study the gas dispersion.

Subsequent research efforts will be put further to address the heavy gas dispersion using multi-species modeling methodology.

References

[1] *User's Guide for the AMS/EPA Regulatory Model – AERMOD*. EPA-454/B-03-001, Environmental Protection Agency, United States, September 2004.

[2] *User Guide of OpenFOAM – The Open Source CFD Toolbox*. version v1612+, OpenCFD Limited.

[3] Patankar S. V., *Numerical Heat Transfer and Fluid Flow*. McGRAW-HILL BOOK COMPLANY, ISBN 0-07-048740-5, 1980.

[4] Gromke C., Buccolieri R.Sabatino S. D. and Ruck B., Dispersion study in a street canyon with tree planting by means of wind tunnel and numerical investigations – Evaluation of CFD data with experimental data. *Atmospheric Environment* 42(37): 8640-8650, 2008.

[5] Chang J. and Hanna S., Air quality model performance evaluation. *Meteorology and Atmospheric Pysics* 87 (2004):167-196.

[6] Biltoft C. A., *Customer Report for Mock Urban Setting Test*. DPG Document No. WDTC-FR-01-121, Dec 2001.

[7] Bekka N., Kumar P., Feiz A., Singh S., Sellam M., Barbosa E., Ngae P., Turbelin G. and Chpoun A., A CFD modeling approach for a contaminant released in a city. *17th Int. Conf. on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*, May 2016, Budapest, Hungary.

[8] Blocken B., Stathopoulos T. and Carmeliet J., CFD simulation of the atmospheric boundary layer: wall function problems. *Atmosheric Environment* 41(2): 238-252.