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New plume rise modeling in a turbulent atmosphere via hybrid RANS-LES numerical simulation

Ali Ahmadi Orkomi [a,*], Khosro Ashrafi [b], Majid Shafipour Motlagh [b]

[a] Department of Environmental Science and Engineering, Faculty of Natural Resources, University of Guilan, Rasht, Iran
[b] Department of Environmental Engineering, Faculty of Environment, University of Tehran, Tehran, Iran

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ABSTRACT

New plume rise formulas are developed to overcome the drawbacks of the conventional models in predicting the rise of buoyant jets in different atmospheric stability conditions. A hybrid Reynolds averaged Navier Stokes (RANS) and large eddy simulation (LES) approach with a mixed scale sub-grid parameterization technique is applied. By using the aforementioned simulation results, new plume rise formulas are derived. The direct effects of atmospheric turbulence intensity at stack height (I_{Air}) and the vertical derivative of wind velocity are introduced in plume rise formulas. The quantile-quantile plots show that new formulas can predict the simulated plume rise in the turbulent crossflow with a deviation factor of 1.18, 1.0025 and 1.17 for stable, neutral and unstable conditions, respectively whereas the conventional models overestimate the final plume rise at least by a factor of 6.1, 3.4 and 2.7. Moreover, by applying the new plume rise formulas in Gaussian dispersion model, the accuracy of new formulas is evaluated. The results show that by applying the new plume rise formulas instead of the conventional Briggs formulas in the Gaussian model, the normalized mean square error reduces by 20% and the fraction of predictions within a factor of two increases by 50%.

1. Introduction

Because of the complicated dynamics of a buoyant jet in a turbulent atmosphere, its trajectory cannot be predicted by a unique universal plume rise model. Over the past half century, a large number of plume rise models have been developed for some specific cases. Some of them have been derived based on the dimensional analysis (Briggs, 1969) and the others are empirical plume rise formulas, which are obtained from field experiments and physical modeling (Moses and Carson, 1968). Beside, integral plume rise models are also developed to predict the centerline trajectory of plumes. Despite several short-comings of integral models such as internal turbulence omission and linear impact of entrainment, modification of basic integral models in different operating conditions is one of the major fields of interest during past decades (Tao et al., 2013; Marro et al., 2014). Pournazeri et al. (2012) modified the conservation equations to consider updrafts and downdrafts in the integral plume rise models. They validated the results with field data. Decrop et al. (2015) studied momentum-dominated and buoyancy-dominated regimes' feature of a two-phase plume. They also modified the coefficients of the integral plume rise models using numerical simulation results. Tohidi and Kaye (2016) studied the effects of power law wind velocity profile instead of a uniform wind velocity on near field behavior of highly buoyant jets in a non-turbulent atmosphere. According to their research, the wind profile has a significant effect on smoke plume behavior in case of low wind velocity. Although the effects of mean flow parameters on plume rise can be studied well by using the mentioned conventional models, the direct effects of atmospheric and plume turbulence are not explicitly considered in the well-known plume rise formulas. Introducing the effects of turbulent parameters on plume rise models in different atmospheric stability conditions is the main goal of this paper. Approaching this goal requires data in various operating conditions. The data gathering in this paper is conducted by the results of a high quality turbulent flow simulation method. The numerical simulation method not only is less expensive than the field study and physical modeling approach, but also is very suitable for sensitivity analysis in various operating conditions. According to Slawson and Csanady (1967), a plume behavior in the atmosphere may be divided into three distinct phases. In the initial phase, self-generated turbulence of plume is dominated. In the intermediate phase, the inertial subrange part of the atmospheric turbulence (convective or shear induced turbulence) has major role in plume dynamics. Finally, energy containing eddies of the atmospheric turbulence are dominated in the last phase. This theory

* Corresponding author.
E-mail address: Orkomi@guilan.ac.ir (A. Ahmadi Orkomi).

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shows that the turbulence in all scales has an important effect on the plume rise. Therefore, in order to have a reliable CFD data, the applied simulation method should be able to predict the role of these turbulent structures properly. So far, direct numerical simulation (DNS) (Muppidi and Mahesh, 2008), Reynolds averaged Navier-Stokes (RANS) (Reynolds, 1895) and large eddy simulation (LES) (Haren and Nieuwstadt, 1989; Decrop et al., 2015) methods are the well-known methods commonly used to simulate the buoyant jets dynamics. The most distinguishing feature of these simulation schemes is their turbulence parameterization approach.

In terms of computational cost, accuracy and turbulence simulation, the DNS and RANS simulation methods are two extremes and LES occupies an intermediate position between them in which the large-scale eddies are directly simulated and the less important sub-grid scale (SGS) dissipative processes are parameterized using sub-grid models (SGM). Most often, LES can predict the unsteadiness and intermittency of the turbulence structure, which is the most important feature of a buoyancy-driven jet. It should be noted that using LES method in a problem with some unimportant zones is not efficient. In addition, in case of strong turbulence, the scale of flow structures near rigid bodies is too small and LES method needs very fine grids, which increase its computational cost as large as DNS (Gimbun et al., 2012). To overcome this drawback, the hybrid method of RANS-LES is developed during the past decade. From the turbulent modeling point of view, the hybrid method switches from RANS to LES in detached zones of walls and in the parts of the problem where the turbulence prediction accuracy is important. A hybrid RANS-LES method with a new mixed scale sub-grid parameterization technique (RL-DMS(β0.5)) has been introduced in our previous work (Ashrafi et al., 2017) to predict the behavior of buoyant jets in a turbulent crossflow. The mentioned simulation method has been validated (Ashrafi et al., 2017) by experimental data in the literature. All unsteady numerical simulations in this paper are conducted by RL-DMS(β0.5) method in ANSYS Fluent software. By statistical analysis of the data obtained from numerical simulations' results, new plume rise formulas are derived for different atmospheric stability conditions. This paper is organized as follows. In the following section, the problem is defined and the governing equations and solution strategy are discussed. In section 3, the plume rise formulas in the stable, neutral and unstable atmospheric conditions are developed by using the numerical simulation results in different operating conditions. Finally, section 4 concludes the paper.

2. Problem definition and solution strategy

To study the effects of independent parameters on plume rise, downwind trajectory and dispersion of the plume materials are numerically simulated using the RL-DMS(β0.5) method in different operating conditions. The gas ejected from the stack is a two-component mixture of air and Helium (as a tracer gas). The plume rise study is divided into two parts. In the first one, the stable atmosphere is studied and the second one is established for the neutral and unstable atmospheric stability conditions.

In the stable atmosphere, the longitude and latitude size of the physical domain is 600 m and 200 m, respectively. In order that the simulation results are not affected by top boundary conditions, the height of the domain varies from 100 m to 180 m corresponding with changes in ABL height. A 16 m carbon steel chimney with an inner diameter of 0.6 m is located 42 m downstream of the inlet boundary. In neutral and unstable conditions, the length and the height of the domain are 900 m and 270 m, respectively. It should be noted that the value of 270 m for domain height in neutral and unstable conditions is a conservative choice, where the effects of boundary conditions on simulation results are not significant in any case study. The stack diameter, height and its longitudinal coordinates multiplied by 1.5 in neutral and unstable conditions.

2.1. Governing equations and solution method

The behavior of a buoyant jet can be predicted by solving the conservation equations of mass, momentum and energy. The hybrid RANS-LES method, which switches to RANS model when the turbulence length scale is small and switches to LES sub-grid scale model in the massive detached regions, is applied for solving the conservation equations. The filtered non-Boussinesq Navier Stokes equations of the incompressible gas mixture using Einstein convention are as below:

$$\frac{\partial(\rho\overline{U}_i)}{\partial x_i} = 0 \tag{1}$$

$$\left[\frac{\partial\rho\overline{U}_i}{\partial t} + \frac{\partial(\rho\overline{U}_i\overline{U}_j)}{\partial x_j}\right] = -\frac{\partial\overline{P}}{\partial x_j} + \rho g_i + \mu\left[\frac{\partial^2(\overline{U}_i)}{\partial x_j^2}\right] - \frac{\partial\tilde{\tau}_{ij}}{\partial x_j} \tag{2}$$

$$\left[\frac{\partial\rho\overline{T}}{\partial t} + \frac{\partial(\rho\overline{U}_j\overline{T})}{\partial x_j}\right] = \frac{k}{c_p}\left[\frac{\partial^2\overline{T}}{\partial x_j^2}\right] - \frac{\partial(\tilde{\tau}_{Tj})}{\partial x_j} \tag{3}$$

$$\left[\frac{\partial(\rho\overline{m}_i)}{\partial t} + \frac{\partial(\rho\overline{U}_j\overline{m}_i)}{\partial x_j}\right] = D_i\left[\frac{\partial^2(\rho\overline{m}_i)}{\partial x_j^2}\right] - \frac{\partial\tilde{\tau}_{m_ij}}{\partial x_j} \tag{4}$$

in which $\overline{U}_i$ is the resolved velocity vector. $\rho, P, g_i, \mu, T, k, c_p, m_i$ and D_i are density, pressure, gravity modulus, dynamic molecular viscosity, temperature, thermal conductivity, mass specific heat capacity, mass fraction of species i and molecular mass diffusivity, respectively. To close the conservation equations, the turbulent stress terms ($\tilde{\tau}_{ij}$, $\tilde{\tau}_{Tj}$ and $\tilde{\tau}_{m_ij}$), which contain the unresolved scales' effects, should be parameterized. According to the Boussinesq hypothesis (Boussinesq, 1877), the turbulent stress terms can be defined as follow:

$$\tilde{\tau}_{ij} - \frac{1}{3}\tilde{\tau}_{kk}\delta_{ij} = -2\mu_T\overline{S}_{ij} \tag{5}$$

$$\tilde{\tau}_{Tj} = -\frac{\mu_T}{\mathrm{Pr}_T}\frac{\partial\overline{T}}{\partial x_j} \tag{6}$$

$$\tilde{\tau}_{m_ij} = -\frac{\mu_T}{Sc_T}\frac{\partial\overline{m}_i}{\partial x_j} \tag{7}$$

where μ_T and $\overline{S}_{ij}$ are eddy viscosity and resolved rate of strain tensor, respectively. Pr_T is the turbulent Prandtl number which is set to 0.85. Sc_T is the turbulent Schmidt number, which is set to 0.3 (Blocken et al., 2008). Although the value of Sc_T is set to 0.3, the effects of different values of Sc_T number on the final plume rise are also studied.

As mentioned above, when the turbulent length scale is small, the mentioned zone is solved by the RANS approach. Because of this, the k-ω turbulent model, which is suitable to consider low Reynolds number effects (Wilcox, 2006), is used in the RANS mode. In the LES region, the SGS turbulent viscosity is estimated via the mixed scale model (Eq. (11)). The turbulent kinetic energy ($\tilde{K}$) and its specific dissipation rate ($\tilde{\omega}$) are solved first by Eqs. (8)–(10) and finally the turbulent viscosity is estimated by Eq. (11).

$$\left[\frac{\partial\rho\tilde{K}}{\partial t} + \frac{\partial(\rho\overline{U}_j\tilde{K})}{\partial x_j}\right] = \mu\left[\frac{\partial^2\tilde{K}}{\partial x_j^2}\right] + \frac{\partial}{\partial x_j}\left[\frac{\mu_T}{\sigma_k}\frac{\partial\tilde{K}}{\partial x_j}\right] + \mu_T|\overline{S}|^2 - \rho\frac{\tilde{K}^{3/2}}{\tilde{l}} \tag{8}$$

$$\left[\frac{\partial\rho\tilde{\omega}}{\partial t} + \frac{\partial(\rho\overline{U}_j\tilde{\omega})}{\partial x_j}\right] = \mu\left[\frac{\partial^2\tilde{\omega}}{\partial x_j^2}\right] + \frac{\partial}{\partial x_j}\left[\frac{\mu_T}{\sigma_\omega}\frac{\partial\tilde{\omega}}{\partial x_j}\right] + \alpha\frac{\tilde{\omega}}{\tilde{K}}\mu_T|\overline{S}|^2 - \beta_i\rho\tilde{\omega}^2 \tag{9}$$