Asymptotic conditions for the use of linear ventilation models in the presence of buoyancy forces

Abstract Low-dimensional discrete linear ventilation models have been studied by Cao and Meyers (2012). In the present study, we investigate the validity and applicability of linear ventilation models for heavy-gas dispersion by employing Reynolds-averaged Navier–Stokes (RANS) simulations. A simple benchmark ventilation case is considered under isothermal condition. Considering large density differences from pollutant gas and fresh air, the effect of buoyancy force has been taken into account in turbulent production term to obtain correct diffusion behaviour. A low- Re k - ε model has been selected and the generalised gradient diffusion hypothesis is used for buoyancy source term. It is concluded that the flow equations decouple from the concentration equation when the ratio α of air mass-flow rate $\dot{m}_a$ to pollutant mass-flow rate $\dot{m}_p$ is larger than 10^5 , which is 10 times higher than the range without density differences ($\alpha > 10^4$). The dependence of the coupling on Richardson number Ri is also studied. It is found that the higher the Richardson number, the larger the α should be to decouple equations.

Key words: linear ventilation models, indoor air-flow, heavy-gas, RANS simulation

INTRODUCTION

Numerical simulation is widely used nowadays for the study of indoor ventilation. The indoor air flow and contaminant distribution in indoor environments are governed by the Navier–Stokes equations combined with a set of species transport equations. Currently, it remains expensive to solve these equations using CFD approaches (DNS, LES, or RANS). Consequently CFD is mainly suited for design purposes, cannot be directly used for online monitoring and control of indoor ventilation. In Cao and Meyers (2012), a low-dimensional discrete linear ventilation model has been elaborated. The model is derived directly from the Navier–Stokes and species transport equations, which allows for a better parameterization of indoor pollutant distribution. The linear model can be used as a fast mathematical model for the online monitoring or control of ventilation systems. Once constructed, we can reconstruct pollutant concentration field from any type on indoor pollutant source distributions.

In previous work, the focus was on the elementary development of discrete low-dimensional linear ventilation models and investigation of related numerical issues. To that end, a simple benchmark ventilation case in a steady-state and constant-density environment was considered. The validity of discrete linear ventilation models for different Reynolds numbers was demonstrated in Cao and Meyers (2011), again for constant-density conditions. However, buoyancy effects can have a large impact on pollutant dispersion.

The presence of buoyancy leads to a volumetric gravitational force term in the momentum equations. Next to that turbulence levels are also influenced. Nowadays, state-of-the-art numerical simulation for ventilation systems control is mainly executed using RANS with k -

ε models, and buoyancy-modified k - ε models have been extensively investigated in the past few years (Chung and Devaud, 2008; Ricciardi et al. 2008; Worthy et al. 2001; Yan and Holmstedt, 1999). In these, the effect of buoyancy force is added as a source term both in turbulent kinetic energy equation, and dissipation equation.

A prerequisite for the construction of linear (low-dimensional) ventilation models, is the requirement that the concentration transport equation decouples from the flow equations (and Meyers 2012). In the current study, we investigate this coupling when density-related gravity effects play a role. In section 2, we briefly describe the decoupling between the concentration and velocity field when the ratio α of air-mass-flow-rate $\dot{m}_a$ to pollutant-mass-flow-rate $\dot{m}_p$ increases to infinity. In section 3, a number of RANS simulations are presented to investigate the asymptotic behavior of ventilation with respect to α . At too low values of α , buoyancy effects start to couple the concentration equation to the flow equations. In this regime concentration distributions cannot be described by linear ventilation models. Finally, conclusions are presented.

RESEARCH METHODS

2.1. Non-dimensional transport equations

A simple ventilation case is considered in an indoor environment (or ‘room’) with an in- and outlet, and a source distribution of gaseous pollutants S_p (see Figure 1, for an outline). The room volume and inlet-vent area are denoted as Ω , and A . For sake of simplicity, we only consider two species, i.e. air, and one type pollutant. At the inlet, fresh air is supplied with an average velocity U_0 , and a density ρ_0 . Inside the room, air and pollutant are mixed,

respectively with mass fraction $1-Y$ and Y . The room conditions are presumed to be isothermal, constant-density, with $\rho = \rho_0$ and steady state.

Figure 1: Outline of a simple indoor-ventilation case

Special strategies are required to generalize the discrete linear ventilation models, which are demonstrated in details in Cao and Meyers (2012). First we need to normalize transport equations by using a suite of reference scales with a reference length $L = \Omega^{1/3}$ (Ω room volume size), a reference velocity U_0 , and a reference density ρ_0 . For the concentration, we use the well-mixed pollutant concentration (the average mass fraction) Y_0 at the ventilation outlet as a reference. Then all transport equations are associated with non-dimensional mass flux ratio α of air mass-flow rates $\dot{m}_a$ to pollutant mass-flow rates $\dot{m}_p$ in the ventilation system ($\alpha \equiv \dot{m}_a / \dot{m}_p$). When the ratio α is sufficiently large ($\alpha \rightarrow \infty$), the flow equations can be decoupled from the pollutant concentration equation (Cao and Meyers, 2012). Here, we

briefly summarize the resulting normalized RANS equations. The RANS continuity, momentum and concentration equations respectively correspond with

$$\nabla^* \cdot (\bar{\rho}^* \tilde{\mathbf{u}}^*) = \frac{K}{\alpha} S_p^*, \quad (1)$$

$$\nabla^* \cdot (\bar{\rho}^* \tilde{\mathbf{u}}^* \otimes \tilde{\mathbf{u}}^*) + \nabla^* \bar{p}^* - \frac{2}{Re} \nabla^* \cdot (1 + \nu_t^*) [S^* - \text{tr}(S^*) I / 3] - Ri \frac{\tilde{C}^*}{1 + \alpha} \frac{\bar{\rho}^*}{\rho_p^*} = 0, \quad (2)$$

$$\nabla^* \cdot (\bar{\rho}^* \tilde{\mathbf{u}}^* \tilde{C}^*) - \frac{1}{Re Sc} \nabla^* \cdot (1 + D_t^*) \nabla^* \tilde{C}^* = \left(1 + \frac{1}{\alpha}\right) K S_p^*, \quad (3)$$

where, $\tilde{\mathbf{u}}^*$ and $\tilde{C}^*$ are time averaged velocity and concentration; ν_t^* , D_t^* are the non-dimensional eddy viscosity and eddy diffusivity, defined as $\nu_t^* = \nu_t / \nu_0$, $D_t^* = D_t / D_0$ respectively, and ν_0 is the viscosity of air, D_0 the mass diffusion coefficient. Further K is a constant ($K = A/L^2$, with A the area of the inlet), S_p^* the non-dimensional pollutant source term, and $S^* = [\nabla^* \tilde{\mathbf{u}}^* + (\nabla^* \tilde{\mathbf{u}}^*)^T] / 2$ the strain rate tensor. Finally, the non-dimensional parameters in equation (1) and (2) are the Reynolds number, Re , Schmidt number, Sc , and Richardson number, Ri :

$$Re = \frac{U_0 L}{\nu_0}, Sc = \frac{\nu_0}{D}, Ri = \frac{g(\rho_p - \rho_0)L}{\rho_0 U_0^2}. \quad (4)$$

Further details and definitions can be found in Table.1. By looking at the non-dimensional forms of the continuity and concentration equations (Equations. 1, 3), it is found for $\alpha \rightarrow \infty$ that

$$\lim_{\alpha \rightarrow \infty} \left[\frac{K}{\alpha} S_p^* \right] = 0; \lim_{\alpha \rightarrow \infty} \left[Ri \frac{\tilde{C}^*}{1 + \alpha} \frac{\rho^*}{\rho_p^*} \right] = 0; \lim_{\alpha \rightarrow \infty} \left[\left(1 + \frac{1}{\alpha} \right) K S_p^* \right] = K S_p^*. \quad (5)$$

Table 1. Summary of terms and expression used in the RANS equations

$\dot{m}_a = \rho_0 U_0 A, \dot{m}_p = \iiint_{\Omega} S_p(\mathbf{x}) d\mathbf{x}, Y_o = \dot{m}_p / (\dot{m}_a + \dot{m}_p) = 1/(1 + \alpha)$
$S_p^* = S_p L^3 / \dot{m}_p, \nu_0 = \mu_0 / \rho_0, D_t = \nu_t / Sc_t$

Hence, for $\alpha \rightarrow \infty$, the solution of the continuity and momentum balance are decoupled from the pollutant concentration $\tilde{C}^*$. Consequently, the pollutant transport equation of $\tilde{C}^*$ becomes a linear-partial-differential equation, which can be solved once the velocity field is known (e.g. based on a set of numerical simulations or experiments). In that case, Green's functions $G(\mathbf{x}, \mathbf{x}')$ can be employed to construct a (low-dimensional) linear ventilation model (details can be found in Cao and Meyers, 2012), i.e.

$$\langle \tilde{C}^* \rangle_{\Omega_c} \approx \sum_{j=1}^M \bar{G}_{cj} S_j^*, \quad (6)$$

where $S^* = K S_p^*$, and where $\bar{G}$ is a square matrix that can be constructed based on a number of precursor flow simulations.

In the current work, we do not focus on the construction of linear ventilation models (6) as such, but rather investigate in more detail the conditions under which they can be used, i.e. we investigate in the presence of buoyancy effects when the concentration equation (3) decouples from the momentum equations (2)

2.2. Turbulence modeling

We investigate the effect of buoyancy caused by density differences. To that end, the buoyancy-modified k - ε models are employed to close Navier-Stokes equations, accompanied with buoyancy source terms in the turbulent transport equations for both turbulent kinetic energy k and turbulent dissipation ε (Chung and Devaud, 2008; Ricciardi et al. 2008; Worthy et al. 2001; Yan and Holmstedt, 1999). k and ε are further elaborated under steady state:

$$\nabla^* \cdot (\bar{\rho}^* \tilde{\mathbf{u}}^* \otimes k) = \frac{1}{Re} \nabla^* \cdot \left(\nu + \frac{\nu_t}{\sigma_k} \right) \nabla^* k + P_k^* - \varepsilon + G_k^*, \quad (7)$$

$$\nabla^* \cdot (\bar{\rho}^* \tilde{\mathbf{u}}^* \otimes \varepsilon) = \frac{1}{Re} \nabla^* \cdot \left(\nu + \frac{\nu_t}{\sigma_\varepsilon} \right) \nabla^* \varepsilon + \frac{\varepsilon}{k} (C_1 f_1 P_k^* - C_2 f_2 \varepsilon + C_3 f_3 \max(0, G_k^*)). \quad (8)$$

where, P_k^* is the turbulent production term, modelled as $P_k^* = \nu_t \nabla^* \tilde{\mathbf{u}}^* : \nabla^* \tilde{\mathbf{u}}^*$, G_k^* is the production of k due to buoyancy effects, and based on eddy diffusivity model,

$$G_k^* = -Ri \frac{1}{1+\alpha} \frac{1}{\rho_p^*} \overline{\rho^* \mathbf{u}^* \cdot \nabla^* C^*} = -D_t^* Ri \frac{1}{1+\alpha} \frac{1}{\rho_p^*} \nabla^* \tilde{C}^* \quad (9)$$

Finally, additional constants Sc_t , C_μ , C_1 , C_2 , C_3 , σ_k , σ_ε , and functions f_μ , f_1 and f_2 are defined in Table 2.

Table 2 Constants and damping functions used in the turbulence model

$[Sc_t, C_\mu, C_1, C_2, C_3, \sigma_k, \sigma_\varepsilon] = [0.9, 0.09, 1.44, 1.44, 1.92, 1.0, 13]$
$f_\mu = [1.0 - \exp(-0.0215 Re_k)]^2 (1 + 31.66/Re_t^{5/4}), f_1 = f_3 = 1.0$
$f_2 = [1.0 - 0.01 \exp(-Re_t^2)] [1 - \exp(-0.0613 Re_k)], Re_k = \sqrt{k} y / \nu, Re_t = k^2 / \nu \varepsilon$

RESULTS AND DISCUSSION

A series of RANS simulations of a simple ventilation benchmark case are performed by using the commercial software ANSYS Fluent 12.1. The case consists of a cubic room with top-left inlet slot, and bottom-right outlet slot. A detail of the geometry, and the computational mesh used for the CFD is provided in Figure 2. The computational mesh is block structured (cf. Fig. 2) containing a total of 1,254,400 cells (i.e. $74 \times 40 \times 80$ cells in the inlet block, $80 \times 152 \times 80$ in the main block, and $20 \times 28 \times 80$ cells in the outlet). The grid is stretched near the wall, and the first grid-point is typically located at a distance of $0.5 \times 10^{-3}L$ from the wall. For the current Reynolds number of 1500, we verified that this ensures a distance from the wall, using inner units, which remains well below $y^+ = 5$, such that the near-wall region is sufficiently resolved to justify the use of the low-Reynolds number $k-\epsilon$ model. A grid refinement study is also performed, with a finer grid using a total of 4,140,000 cells (compared to 1,254,400 for the baseline case). We find that the baseline case is sufficiently resolved, with differences of velocity and turbulent kinetic energy between the two grid cases remaining below 3% (results are not further shown here).

Figure 2. Computational set up of the indoor-ventilation test case

Figure 3. Contours of dimensionless air flow velocity, and pollutant concentration at xy -plane ($z=0.5L$). (a) Velocity field from RANS simulation; (b) Concentration field $\tilde{C}^*$. In (a) and (b), the pollutant-source is marked with $\bullet$, and streamlines are also shown

At the inlet, a uniform velocity profile is given. The turbulence intensity is set at 1%, and a turbulent length scale of $1 \times 10^{-4}L$ is chosen (i.e. equal to the upstream mesh-opening size in the screens of corresponding experimental set-up at Eindhoven University of Technology). Based on definition of Re and Ri in section 2, the magnitude of each is corresponding to 30,000 and 200. At the outlet, a standard pressure-outlet condition is used. No-slip boundary conditions are set for all walls. The non-dimensional ventilation equations are solved in RANS formulation, and solved with a low-Reynolds number $k-\varepsilon$ model of Chang et al. (1995). We choose this model because it is able to predict the correct behavior of the free-stream turbulence coming from the contraction part of the geometry, and yields a good prediction of velocity fields inside the enclosure when compared to PIV experiments (Cao and Meyers, 2013).

3.1. The distribution of flow field and pollutant field in ventilated enclosure

In Figure 3 (a,b) the distribution of velocity and concentration at xy -plane ($z=0.5L$) obtained from the simulation is presented. It is shown that the velocity profile has a large impact on the eventual distribution of pollutants in the ventilated enclosure. The entering of fresh air into the room can be taken as the evolution of the wall jet. Generally speaking, the flow in the ventilated enclosure is classified into three region, free jet, Coanda effect, and wall jet region (Awbi, 2003; Hooff, T.A.J. van, et al., 2012). When the free jet enters into room, it remains attached to the ceiling due to Coanda effect until its separation and it moves downwards along the side wall. The jet then separates and reattaches to the wall at the every corner. Since the pollutant source is located in the primary recirculation region, the pollutant is transported following this primary recirculation and moving towards the flow direction to about $y=0.9L$ then downward and toward the ventilation exit. Turbulent mixing happens along the flow trajectory between the primary recirculation and secondary recirculation region, which allows for part of pollutant entering into the secondary recirculation. Therefore, pollutant in the primary recirculation is transported either to the ventilation exit through turbulent mixing processes with fresh air or recirculated back inside domain. It is further noticed that in Figure 3(b) a placement of the pollutant point-source in a region of low velocity leads to peak concentrations $\tilde{C}^*$ in the room of over 10 (relative to the well-mixed concentration at the outlet).

3.2. The density effects on asymptotic behavior for $\alpha \rightarrow \infty$ of indoor ventilation

We now investigate the effect of buoyancy on the coupling of the concentration equation to the flow equations. To that end, we consider 12 RANS simulations that include 11 different finite indoor α magnitudes ranging from 10^3 to 10^6 and an infinite one $\alpha=\infty$ (representing the decoupled case).

Figure.4 The dependence on the presence of buoyancy effects of relative recirculation R (a), and locally averaged maximum concentration (b) in ventilated enclosure with respect to α for different point-source locations; values are displayed relative to the asymptotic value R_∞ ; in (b), $\langle \tilde{C}^* \rangle_{max}$ is the maximum of locally averaged concentration over an averaging volume with size $(0.1L)^3$ [Symbols:(*): Point A and ($\square$): Point B]

Two scenarios with a different location of pollutant point sources inside the ventilated enclosure are considered, i.e. one case that is located respectively at well ventilated area (Point A $(x,y,z)=(0.7,0.3,0.3)L$) and another with a source at poorly ventilated area (Point B $(x,y,z)=(0.5,0.3,0.3)L$). To investigate the dependence of linear ventilation model on the range of α , two ventilation parameters are selected, which are relative recirculation rate R and averaged peak concentration $\langle \tilde{C}^* \rangle_{max}$. $\langle \tilde{C}^* \rangle_{max}$ is the concentration locally averaged over a volume Ω_L normalized by its corresponding asymptotic values when $\alpha \rightarrow \infty$, and we take one averaging size, i.e. $\Omega_L=(0.1L)^3$. For both ventilation parameters, the asymptotic behavior happens at the same range of α ($\alpha > 10^5$) shown in Figure 4. Then we can decouple pollutant concentration equation from flow Navier-Stokes equations, which can be served for the

Figure.5 The dependence on Richardson number effects of relative recirculation R (a), and locally averaged maximum concentration (b) in ventilated enclosure with respect to α for point-source located at $(x,y,z)=(0.5,0.3,0.3)L$; values are displayed relative to the asymptotic value R_∞ ; in (b), $\langle \tilde{C}^* \rangle_{max}$ is the maximum of locally averaged concentration over an averaging volume with size $(0.1L)^3$ [Symbols:(*): $Ri=50$; ($\square$): $Ri=200$; ($\diamond$): $Ri=400$:]

application of linear ventilation model. It is appreciated that this conclusion is corresponding to rough estimates in previous research work that effects of gravity (density differences) leads to conditions on α that are a factor of 10 higher than the range for isodensity cases ($\alpha > 10^4$) (Cao and Meyers, 2012).

It is further observed that the differences of both ventilation parameters R and $\langle \tilde{C}^* \rangle_{max}$ with respect to the asymptotic values at $\alpha=\infty$ reach levels up to 70%. Hence, the buoyancy effects are playing a very important role in turbulent diffusion when the magnitudes of α are low. The dependence of the coupling on Richardson number is also studied by employing a suite of RANS simulations with different indoor Ri magnitudes (50, 200, 400). From Figure 5, it is

appreciated that the asymptotic behavior of both parameters of R and $\langle \tilde{C}^* \rangle_{max}$ depends on Richardson number. At low values $Ri = 50$, $\alpha > 4 \times 10^4$ may already be fine. For $Ri = 400$, asymptotic behavior is observed for $\alpha > 10^5$.

CONCLUSIONS

This work discussed the coupling issue between Navier-Stokes equations and pollutant transport equation with density effects (buoyancy/gravity effects). When gravity effects are taken into account, it was demonstrated that the flow equations decouple from the concentration equation while the ratio α of air mass-flow rate $\dot{m}_a$ to pollutant mass-flow rate $\dot{m}_p$ is larger than 10^5 , which is 10 times higher than the range without density differences ($\alpha > 10^4$). Hence, under these conditions, (low-dimensional) linear ventilation models can be constructed as documented in Cao and Meyers (2012). For lower values of α , buoyancy effects are of importance in the coupling between the pollutant transport equation and the flow equation. Further research is required to investigate how in that case buoyancy effects can be taken into account into low-dimensional ventilation models.

The study in the current manuscript is based in a relatively simple cubical room without obstructions, and is meant to serve as a first case for the illustration of the principles underlying linear ventilation models. However, the extrapolation of the asymptotic results for α to more realistic ventilation geometries should be performed with caution. For instance, in scenarios where sub-regions in the ventilated enclosure are ‘almost’ separate from the main domain, or where large pockets of laminar quiescent air exist, extrapolations may become problematic. In many other situations, results obtained here, may serve as a first order-of-

magnitude estimate. Obviously, this should be further corroborated with an elaboration of more complex ventilation cases. This is subject of future research work.

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