Title: Simulation of Non-Passive Particle Dispersion in Ventilated Rooms

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Synopsis
Concentrations of indoor air contaminants are normally calculated by assuming that they fully follow airflow paths in a room. This assumption is also used to predict the local residence time of contaminants in a room, which may further be used to characterise the ventilation effectiveness. In this paper, a different methodology has been adopted, in which indoor airborne particles do not always follow the main airstream induced by the ventilation system. Dispersion of particles is predicted by a drift-flux model. The model assumes that the settling velocity of each particle is sufficiently small when compared to the high inflow velocity and the volumetric concentration of particles is also very low. This assumption has justified the use of a drift-flux multi-phase model rather than a fully coupled multi-fluid model. Additionally, the effect of the particles on turbulence can be neglected. In the drift-flux model, a settling term is added to the concentration equation, and the body force term in the momentum equation is treated using the principle of a Boussinesq approximation, similar to that in a thermal-buoyancy-driven flow.

The model has been previously validated by comparing numerically calculated results with those measured in an aerosol chamber. In the examples in this paper, particles with diameters ranging from 0.5 \( \mu m \) to 5 \( \mu m \) are supplied into a room through a ventilation and air-conditioning register. Local particle concentrations are calculated for different particle size groups. It is shown that in the air-conditioning situations considered, the thermal-buoyancy-introduced flows provide an additional mixing mechanism for particle dispersion in the room. The developed model can be a useful tool for minimising particle concentrations in the air by evaluating and selecting an optimum air distribution and air-conditioning system.

1. Introduction
Contaminant and particle concentrations have often been used as a direct measure of indoor air quality in buildings. In ventilation and industrial hygiene, many design guidelines and regulations specify the threshold of a particular contaminant concentration. Thus, there has been considerable interest in the literature in attempting to predict the contaminant concentration and turbulence dispersion of contaminants and particles. Indeed, the particle concentration is closely related to the flow pattern in a flow system. In the 1950's, a tracer concentration history in a flow system was used to introduce the concepts such as residence time and age of the fluids in chemical engineering. These concepts have been further developed in the field of ventilation to evaluate ventilation performance. In ventilation engineering, one very useful modification to the concentration equation is the steady state transport equation for the mean age of the air (see for example [1] and [2]). In all the situations considered, the particles of the tracer are assumed to be passive, i.e. they follow the airflow path in an enclosure.
In this paper, a new concentration equation is suggested for non-passive (settling) particles. By modifying the general concentration and momentum equations, particle settling velocities can be considered when movement of indoor air pollutants in rooms is simulated. This allows the settling rates of dust and other solid pollutants to be estimated.

The new model, where air velocity turbulence is calculated by a k-ε model, is expected to give a better understanding of the relationships between room geometries, ventilation airflow rates and ventilation principles on one hand, and pollutant characteristics and concentration levels on the other. Simulations can be used to find the optimal air distribution principle to eliminate/minimise identified harmful indoor air particles in built environment. A particular area of interest is the human near-body zone, where the particle behaviour and local concentrations are of particular importance from an occupational health point of view. The work to be presented in this paper has been a close collaboration between the two authors who represent two separate organisations with a strong interest in dust and pollutant control.

2. Governing equations for particle dispersion

The general governing equation for continuity and transport is:

$$\frac{\partial (\rho u_j \varphi)}{\partial x_j} = \frac{\partial}{\partial x_j} (\Gamma \frac{\partial \varphi}{\partial x_j}) + S.$$  \hspace{1cm} (1)

where subscript $j$ stands for coordinate directions. The equation components are given in Table 1. From Equation (1) the z direction momentum equation is given by:

$$\frac{\partial (\rho u_j w)}{\partial x_j} = \frac{\partial}{\partial x_j} (\Gamma \frac{\partial w}{\partial x_j}) + S + F_{\Delta \rho} + F_{\Delta T}$$  \hspace{1cm} (2)

where body forces due to particle/fluid density differences ($F_{\Delta \rho}$) and thermal differences ($F_{\Delta T}$) are modelled by using a Boussinesq approximation. A particle settling velocity $w_s$ is included in the concentration equation, giving the following equation for concentration calculations of non-passive particles in the air:

$$\rho (u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + (w + w_s) \frac{\partial c}{\partial z}) = \frac{\partial}{\partial x} (\Gamma \frac{\partial c}{\partial x})$$  \hspace{1cm} (3)
Table 1. General transport parameters for Equation (1). The pressure component is given by $p$, temperature by $T$, laminar Prandtl number (Schmidt number) by $\sigma$, fluid viscosity by $\mu$ and density by $\rho$. Subscripts $c$, $i$ and $t$ indicate concentration, coordinate direction and turbulence.

<table>
<thead>
<tr>
<th>EQUATION</th>
<th>$\varphi$</th>
<th>$\Gamma$</th>
<th>$S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Momentum</td>
<td>$u_i$</td>
<td>$\mu + \mu_i$</td>
<td>$- \partial p/\partial x_i$</td>
</tr>
<tr>
<td>Particle concentration</td>
<td>$c$</td>
<td>$\mu/\sigma + \mu_i/\sigma_i$</td>
<td>0</td>
</tr>
<tr>
<td>Energy</td>
<td>$T$</td>
<td>$\mu/\sigma + \mu_i/\sigma_i$</td>
<td></td>
</tr>
<tr>
<td>Turbulent kinetic energy</td>
<td>$k$</td>
<td>$\mu + \mu_i/\sigma_k$</td>
<td>$P_k - \rho \varepsilon$</td>
</tr>
<tr>
<td>Dissipation of $k$</td>
<td>$\varepsilon$</td>
<td>$\mu + \mu_i/\sigma_k$</td>
<td>$\varepsilon(C_{e_1}P_k - C_{e_2}\rho \varepsilon)/k$</td>
</tr>
</tbody>
</table>

For non-isothermal calculations (the air-conditioning case), the temperatures of all wall surfaces were 25°C and that of the supply air was 17°C. The standard $k$-$\varepsilon$ turbulence model [3] was used together with wall functions for near-wall grid points. The boundary conditions for the $k$-$\varepsilon$ turbulence model used at supply registers are determined by using an assumption of the isotropic turbulence. This gives the following boundary condition for the supply turbulent kinetic energy [4], $k$:

$$k = \frac{3}{2} I^2 u^2$$  \hspace{1cm} (4)

where $I$ is the supply turbulence intensity and $u$ is the supply velocity.

The energy dissipation rate, $\varepsilon$, is given by:

$$\varepsilon = 0.1643 \, k^{1.5}/d$$  \hspace{1cm} (5)

where $d$ is the supply inlet diameter. At the outlet a zero streamwise gradient is prescribed, i.e.:

$$\frac{\partial u_i}{\partial x} = \frac{\partial T}{\partial x} = \frac{\partial c}{\partial x} = \frac{\partial k}{\partial x} = \frac{\partial \varepsilon}{\partial x} = 0$$  \hspace{1cm} (6)

where $x$ is the coordinate direction normal to the outlet.
4. Model evaluation
A preliminary validation of the numerical particle dispersion model has been reported by the authors in a previous paper, [5]. Briefly, the validation was carried out by comparing numerically calculated velocity profiles and particle settling on wall surfaces with those measured in an aerosol chamber. The use of a drift-flux model for predicting particle dispersion has also been demonstrated for a liquid-solid separation problem in an industrial vessel, [6].

5. Application and results
A finite volume computer code Ventair 1 was used in the present three-dimensional numerical simulations, [7]. For moderate computing times, a grid of (32x22x22) was used in the ventilation and air-conditioning examples to be presented here. A second-order QUICK scheme is used for discretising the convection terms in the momentum equations, and a first-order hybrid scheme is used for discretising the convection terms in the k, ε and concentration equations. The room configuration used for all calculations here is shown in Figure 1.

Figure 1. Room configuration showing geometries and locations of air and particle supply and exhaust.

Particle settling for the flow situation in Figure 2 are given in the Figures 3-5, which show the behaviour of particles with three different aerodynamic diameters (0.5 μm, 2.0 μm and 5.0 μm).
Figure 2. Isothermal velocity field in the middle of the room (x-z). Low air flow velocities in the low-left recirculation zone allows settling of airborne particles. Supply velocity, $u = 1 \text{ m/s}$.

Figure 3. Settling of $5 \mu\text{m}$ particles in an isothermal ventilation situation with recirculation.

Figure 4. Settling of $2 \mu\text{m}$ particles in an isothermal ventilation situation with recirculation.

Figure 5. Settling of $0.5 \mu\text{m}$ particles in an isothermal ventilation situation with recirculation.
According to the numerical results, areas of high pollutant concentration were found where air slowly recirculates. In these low air velocity regions, particles have a chance to settle and higher concentrations than room mean concentrations resulted. Larger particles settle easily, while smaller particles tend to be mixed, as expected. It should be noted here that the particle deposition at wall surfaces was modelled as a perfect deposition situation, i.e. once a particle goes to a wall, it becomes a part of the wall.

**Air-conditioning**

An isothermal case may be ideal in realistic ventilation applications. The presence of thermally driven flows has been shown to produce additional mixing in a room. The most important basic natural convection airstreams are boundary layer flows along wall surfaces and plumes above a heat source. In the mixing ventilation system considered in this paper, natural convection airstreams are generally used, if possible, to interact with the dominant air supply jets to improve the mixing effectiveness. A further numerical test is carried out to study the effect of such a mixing flow system on particle dispersion.

The supply air temperature is assumed to be 17°C, while all wall surfaces are assumed to be 25°C. The wall natural convection flows and the relatively cold supply air have modified the flow pattern significantly (see Figure 6). This has resulted in a flow pattern with less low velocity recirculation and, as a result, almost no settling of particles in the room occurred even for the largest particles considered (see Figure 7).

![Figure 6. Non-isothermal flow pattern with a 17°C air supply temperature and 25°C wall surface temperatures.](image)

![Figure 7. Constant (relative) local concentrations of 5 μm particles in the room. Non-isothermal ventilation (air-conditioning) with cold air supply and warm room surfaces.](image)
The non-isothermal flow was here more efficient than the isothermal flow in removing particles from the room. The absence of stagnant airflow zones has minimized the particle settling and resulted in an unvaried particle concentration in the room. The particle settling situations may be very different in a room ventilated by displacement, as mixing is minimized in the occupied region in that system. A future study will be carried out on displacement ventilation systems.

6. Conclusions

A drift-flux model is used to simulate non-passive particle dispersions in a ventilated (air-conditioned) room. The model assumes that the settling velocity of each particle is sufficiently small when compared to the high inflow velocity and the volumetric concentration of particles is also very low. A settling term is added to the concentration equation, and the body force term in the momentum equation is treated using the principle of a Boussinesq approximation, similar to that in thermal-buoyancy-driven flows.

Particles with diameters ranging from 0.5 \( \mu m \) to 5 \( \mu m \) are supplied into the room through a ventilation and air-conditioning supply register. It is shown that in the isothermal case, particle settling occurs in the low velocity recirculating zone for larger particles. In the air-conditioning case, the additional mixing effect introduced by natural convection flows along wall surfaces provides an efficient flow pattern for removal of all sizes of particle considered.

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