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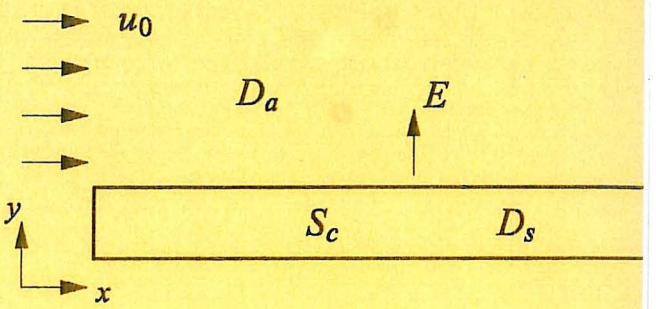

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Paper No 97

Indoor Environmental Engineering

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MODELLING EMISSION FROM BUILDING MATERIALS WITH COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT

This paper presents a numerical model that by means of computational fluid dynamics (CFD) is capable of dealing with both pollutant transport across the boundary layer and internal diffusion in the source without prior knowledge of which is the limiting process. The model provides the concentration distribution in the room air as well as in the source.

The results show that for a given air velocity over the source the concentration of pollutants in the boundary layer is independent of source diffusion coefficient. For evaporative emission, i.e. high source diffusion coefficient, the concentration in the source is decreased as the velocity is increased. In case of internal diffusion being the limiting process the concentration in the source is independent of velocity.

The model predictions have been compared to experimental results and good agreement has been achieved.

INTRODUCTION

Nowadays people spend the majority of their time indoors and it is thus of great importance that buildings provide a healthy, safe and comfortable indoor environment. However, in many new buildings people report a decreased acceptability of the indoor air quality, irritation of mucous membranes and general symptoms such as fatigue and headache often caused by volatile organic compounds (VOC). Due to the large surface area and permanent exposure building materials and furnishings have been identified as major sources of VOC emissions [1, 2].

In general, emission processes involve both diffusion through the material and evaporation from the surface but they are often considered as either evaporative or diffusion-controlled depending on which of the two processes is the limiting. Emission of VOCs from carpets and other flooring materials is mainly controlled by internal diffusion while emission from freshly applied liquid films is typically evaporative. After an initial period of evaporation the emission from a liquid film becomes diffusion-controlled.

Evaporative emission is a function of local airflow parameters such as concentration, temperature, relative humidity, velocity and turbulence while diffusion-controlled emission depends on material properties such as the diffusion coefficient and the material structure. The emission though, always involves mass transfer across the boundary layer along the surface.

At the surface-air-interface the emission rate, E, is often expressed in terms of the mass transfer coefficient, k_c

$$E = k_c(c_w - c_0) \tag{1}$$

where E is the emission from the surface, k_c is the mass transfer coefficient, c_w is the surface concentration, c_0 is the concentration outside the boundary layer.

The diffusion of pollutants within a solid material is analogue to solid heat conduction and is described by Fick's laws for one-dimensional mass transfer

$$J = -D_s \frac{\partial c}{\partial y} \tag{2}$$

$$\frac{\partial c}{\partial t} = D_s \frac{\partial^2 c}{\partial y^2} + S_c \tag{3}$$

where J is the mass flux through the source, D_s is the source diffusion coefficient, c is the concentration, y is the coordinate across the source, t is the time and S_c is the rate at which pollutants are generated in the source.

In the present work a general model by means of computational fluid dynamics (CFD) for emission from building materials is proposed. The model is capable of dealing with pollutant transport across the boundary layer as well as internal diffusion without prior knowledge of which is the limiting process. The model is general applicable as no particular source or pollutant has been studied and it provides detailed information on the pollutant distribution in both the room air and the source. A specific model for VOC emission from a carpet has been demonstrated by Yang, Chen and Bluyssen [3].

It has further been the objective to investigate the influence of surface air velocity and source diffusion coefficient on the concentration distribution in a ventilated room. The model predictions have also been compared to experimental results obtained by Meininghaus, Knudsen and Gunnarsen [4].

METHODS

The computational domain considered in CFD calculations for ventilated rooms is traditionally defined by the physical boundaries of the room. In the present work the computational domain is extended into the pollutant source and the transport equations are solved in the source and the room simultaneously. All CFD calculations have been performed with the commercial software package CFX-4.2. To account for turbulent flow a Low Reynolds Number formulation of the k-ε turbulence model [5] has been applied.

A series of CFD calculations have been performed for steady state air flow over a hypothetical pollutant source to investigate the influence of source diffusion coefficient, D_s, and air velocity on the concentration distribution (see Figure 1).

The pollutant source has been modelled as a solid body in which pollutants are generated at a constant rate per unit volume. In the calculations the free stream velocity, u_0, and the source diffusion coefficient, D_s, have been varied while Sc=1 mg/m^3, D_a=15.1E-6 m^2/s and d=0.02 m.

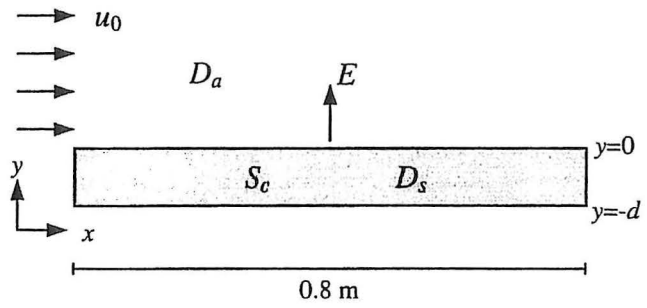

Figure 1. Model for flow over a source with an internal generation of pollutants. u_0 is the free stream velocity, D_a is the air diffusion coefficient, E is the surface emission, S_c is the rate at which pollutants are generated in the source, D_s is the source diffusion coefficient, d is the source thickness and x and y are cartesian coordinates.

Model predictions have further been compared to the results from an experimental study performed by Meininghaus, Knudsen and Gunnarsen [4]. The experimental set-up [4] consisted of a pair of test chambers with a solid material in between (see Figure 2). The primary chamber had a constant supply of polluted air while the secondary chamber was ventilated by clean air.

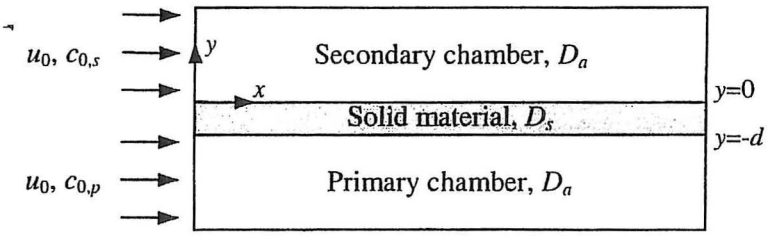

Figure 2. Model for prediction of diffusion through a solid material between two test chambers. u_0 is the inlet velocity, $c_{0,s}$ is the inlet concentration to the secondary chamber, $c_{0,p}$ is the inlet concentration to the primary chamber

RESULTS

It should be noticed that the pollutants assume a solid phase in the source and a gas phase in the air. Henceforward all concentrations are given in terms of the gas phase concentration.

Flow over source with constant internal generation rate

In the following the CFD calculations are evaluated at the middle of the source, that is 0.4 m from the leading edge.

At a given free stream velocity there are large concentration variations within the source while the concentrations in the boundary layer are identical. This is illustrated in Figure 3 where the concentration distribution is shown in logarithmic scale for different source diffusion coefficients.

For low values of D_s, i.e. diffusion-controlled emission, the transport of pollutants through the source is slow and the concentration level is higher than in case of evaporative emission. In

case of evaporative emission there is no significant drop in concentration at the surface as pollutants diffuse quickly through the source.

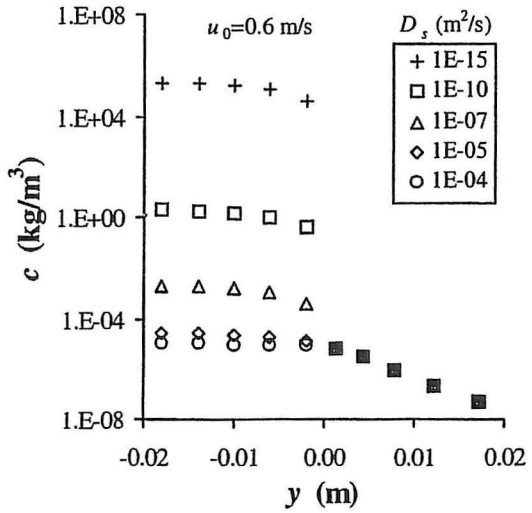

Figure 3. Concentration distribution in logarithmic scale for $u_0 = 0.6$ m/s.

The situation corresponds to heat conduction in a solid with constant thermal load. For low thermal conductivity (low diffusivity) the temperature in the solid will be higher than in a solid with high thermal conductivity.

In Figure 4 and Figure 5 the concentration distribution is shown in logarithmic scale for different free stream velocities at a given source diffusion coefficient.

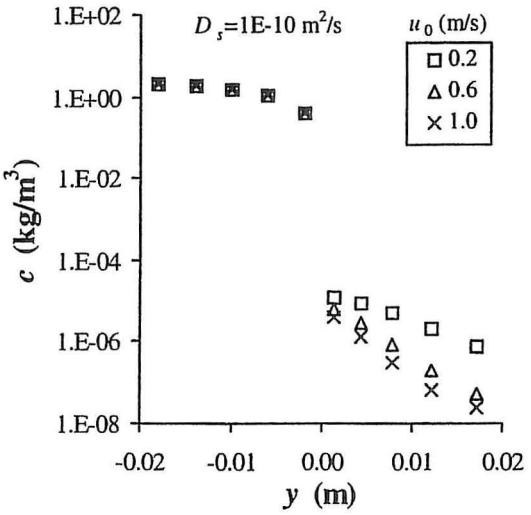

Figure 4. Concentration distribution in logarithmic scale for D_s=1E-10 m²/s.

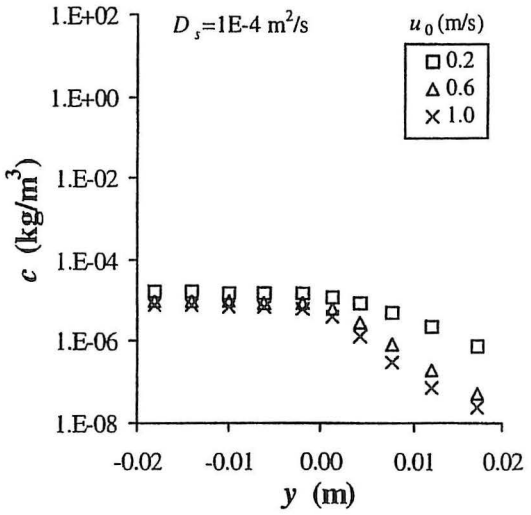

Figure 5. Concentration distribution in logarithmic scale for D_s=1E-4 m²/s.

For D_s=1E-10 m²/s the emission is limited by internal diffusion and the concentration within the source is independent of free stream velocity. The boundary layer concentration though is a function of velocity. The emission is evaporative at D_s=1E-4 m²/s and hence the concentration in both the source and the boundary layer decreases as the velocity increases.

In Figure 6 the mass transfer coefficient is shown as a function of free stream velocity with the source diffusion coefficient as parameter.

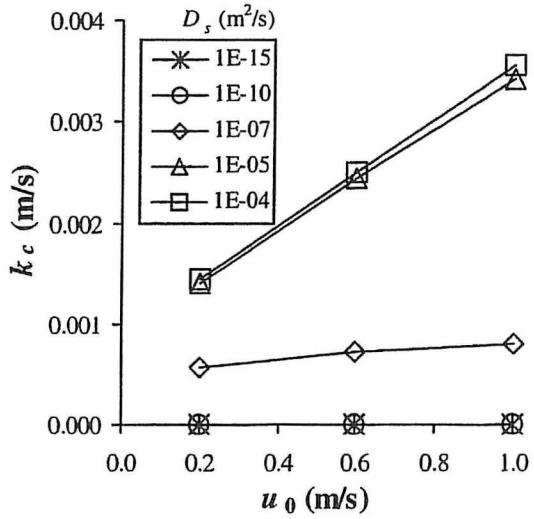

Figure 6. The mass transfer coefficient as a function of free stream velocity.

For low values of D_s the mass transfer coefficient is constant with the free stream velocity but as D_s increases the mass transfer coefficient becomes dependent of the velocity. In other words, the mass transfer coefficient is unaffected by velocity for diffusion-controlled emission but is strongly affected by the velocity when the emission is evaporative.

Prediction of diffusion through a solid material between two test chambers

Figure 7 shows the predicted concentration profiles in the test chambers for diffusion through brick wall (d=25 mm) and aerated concrete (d=21 mm). It is seen that there exists a boundary layer along the material surface as the concentration changes from its surface value to the bulk concentration with in a thin layer.

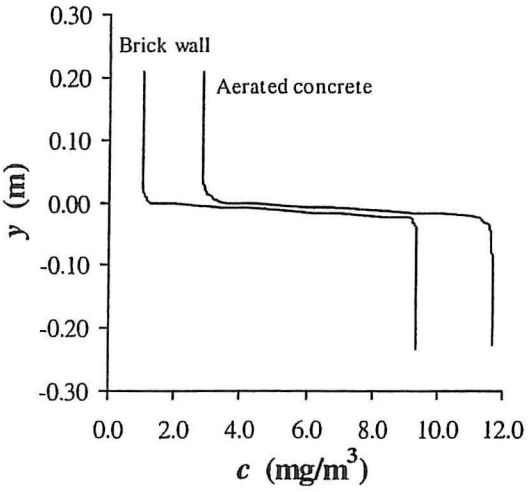

Figure 7. Concentration distributions in the test chambers.

Sample material	Experiment (mg/m³)	CFD (mg/m³)
Brick wall	1.03	1.03
Aerated concrete	2.86	2.85

Table 1. Comparison of measured [4] and predicted exhaust concentrations from the secondary chamber.

Good agreement between the measured [4] and predicted exhaust concentrations from the secondary chamber have been achieved as seen in Table 1. It should be noticed though, that the CFD predictions are based on source diffusion coefficients and inlet concentrations obtained from the experiments.

DISCUSSION

A general applicable numerical model by means of CFD for prediction of emission from building materials in ventilated rooms has been proposed. The model provides detailed information on the concentration distribution in the room air as well as in the pollutant source.

For a source with constant internal generation of pollutants the results show that the mass transfer coefficient is independent of velocity for a diffusion-controlled emission but depends strongly on velocity when the emission is evaporative. The results for the evaporation-controlled emissions are consistent with those obtained by Topp, Nielsen and Heiselberg [6] and Topp et al. [7].

The model has been applied to an experimental set-up and good agreement has been achieved between the measured and predicted concentrations.

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