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A comparative analysis of mathematical models for relating indoor and outdoor toxic gas concentrations in accidental releases

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ABSTRACT

This paper surveys various models for estimating indoor concentration as a function of outdoor concentration in the event of an accidental release or chemical attack involving toxic substances. It is essential to know indoor concentration in order to estimate the effectiveness of shelter in place as a protective measure. Several models—deposition, one-sink, sink-diffusion and two-sink—were considered. These models can be derived from a general model by making different assumptions. The models showed significant variations in terms of the adsorption/desorption considerations. Since indoor materials act as reservoirs, adsorption may lead to a significant decrease in indoor concentration, but subsequent desorption may also take place. The models require the knowledge of a set of parameters that are specific to each compound and material, which are currently scarce in the literature. As a result, the more complex and complete the model, the more limited its applicability.

Outdoor concentrations obtained from a Gaussian model and originating from three source types (continuous, temporary and instantaneous) were used as inputs in the reviewed models. Indoor concentrations of chlorine and sarin from a temporary source were estimated in order to compare the predictions of the models.

1. Introduction

Toxic gas clouds can be caused by a variety of events, including accidental releases on industrial premises, accidents during the transportation of hazardous materials, and attacks involving chemical warfare agents. When a toxic plume appears, one usual protection measure is to shelter in a building and wait until the plume has passed. Evacuation would involve exposure to the toxic release. Since most people spend most of their time inside buildings, they are advised to stay indoors, where the concentration of the toxic substance is supposed to be lower than it is outside. Thus, people are exposed to lower doses of the substance (Chan, Price, Gadgil, & Nazaroff, 2004; Glickman & Ujihara, 1990; Jetter & Whitfield, 2005; Karlsson, 1994; TNO, 1989, chap. 6; Yuan, 2000). Doses are estimated on the basis of the relationship between inside and outside concentrations as a function of time. This paper surveys this relationship for the models analyzed.

Studies in the field of technological risk have focused more on developing models for estimating the outdoor dispersion of neutral and heavy gases in the event of a toxic release than on developing models for relating indoor concentration to outdoor concentration. Indoor concentration is often determined by a mass balance without taking into account indoor processes (i.e. reactions, sorptive interactions with indoor materials, etc.) that can increase or decrease the concentration. Processes of this type have received more attention in the field of indoor air quality where outside concentration is seldom assumed to follow a predefined behavior. In this paper, indoor concentration is related to outdoor concentration using a single model that includes several sorption processes. The paper also evaluates the solutions of various models by using the Gaussian dispersion model to estimate outdoor concentration for cases of continuous and instantaneous releases.

Indoor concentration models were originally developed as a means of estimating the indoor concentration of common pollutants that affect indoor air quality (i.e. CO_2, ozone, VOCs, etc). One of the first models was proposed by Shair and Heitner (1974). This model uses the approximation of a well-mixed chemical reactor and develops a case study of ozone by using a sinusoidal input and a ramp input to simulate outdoor concentration. Recent research in this area has essentially focused on the effects that sorptive interactions between gases and indoor materials have on concentration. Won, Corsi, and Rynes (2001), for example, studied the interactions between eight VOCs and various indoor materials (e.g. carpet, gypsum board, upholstery, vinyl and wood flooring, acoustic tiles, and fruit). They obtained the adsorption/desorption

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rate parameters and analyzed the relationship between the properties of the compounds and the extent of the sorption. Meininghaus, Gunnarsen, and Knudsen (2000), Meininghaus, Salthammer, and Knöppel (1999) and Van Der Wal, Hoogeveen, and Van Leeuwen (1998) ranked indoor materials in different ways, depending on the sink properties for the VOCs analyzed. Several studies have investigated variations in temperature and found that low temperatures favor adsorption (Van Der Wal et al., 1998; Zhang, Zhang, & Chen, 2002; Zhang, Zhang, & Chen, 2003). Jørgensen, Dokka, and Bjørseth (2000) introduced a sink-diffusion model based on adsorption and desorption on, and diffusion into materials. They validated the model using experimental α-pinene and toluene concentrations in a chamber with two types of carpet. Singer, Revzan, Hotchi, Hodgson, and Brown (2004) and Singer, Hodgson, Hotchi, et al. (2005) carried out sorption experiments with several VOCs in furnished rooms, bedrooms and bathrooms. They then fitted the measured concentrations to three sorption models (i.e. one-sink, sink-diffusion and two-sink models) in order to determine the simplest formulation required for each compound. Other authors have analyzed the sink effect of single and combined materials when exposed to a VOC or to a mixture of VOCs (Jørgensen & Bjørseth, 1999; Van Der Wal et al., 1998), and found that sink strength is increased in both cases.

Several models have been used to relate outdoor concentration to indoor concentration with the aim of assessing the effectiveness of shelter in place in the event of the dispersion of toxic gases, chemical warfare substances or biological agents. To evaluate the protective effects of buildings, Karlsson (1994), Karlsson and Huber (1996) and Singer, Hodgson, Destaillats, et al. (2005) analyzed the influence that indoor deposition and desorption of toxic substances had on indoor concentrations. In the assessment of incidents involving biological weapons, Yuan (2000) considers this technique as a protective action, discussing the aspects related to indoor and outdoor concentrations of biological agents.

The TNO (1989, chap. 6) developed a method for relating indoor and outdoor concentrations for three types of sources (i.e. continuous, temporary and instantaneous) in order to evaluate the protection against toxic substances provided by remaining indoors. Casal, Planas, and Casal (1999) assessed sheltering in the event of the spread of an airborne virus. Like the TNO, these authors analyzed the relationship between indoor and outdoor concentrations for continuous, temporary and instantaneous sources and applied them to a case of foot-and-mouth disease in pigs.

Although the models that relate outdoor concentration to indoor concentration can be applied to any gas, the behavior of the outdoor concentration of a toxic gas, when caused by an accidental release, is different from that of the common atmospheric pollutants that are usually present in the atmosphere. Accidental releases have a single source and last for a short period of time (typically less than 60 min). The concentration of the toxic gas downwind from the source is therefore usually computed using a dispersion model that assumes constant atmospheric parameters (e.g. atmospheric stability, wind direction, etc.). Under these conditions, the outdoor concentration profile would be expected to increase and then decrease. In the analysis presented here, the above considerations were taken into account when the outdoor concentration was estimated, and a fairly homogeneous concentration distribution was assumed inside the building when the indoor concentration was calculated (TNO, 1989, chap. 6).

2. General model

Mathematical models for estimating indoor concentration are based on a mass balance that assumes perfect mixing between fresh and inside air (Fig. 1). Since this approach represents a homogeneous concentration distribution, it is commonly applied to single-family residences, since they lack the complexity of multi-family residences or multi-story office buildings (ASHRAE, 2005, chap. 27). As shown in Fig. 1, the most complex case considers pollutants entering along with air due to infiltration and mechanical ventilation; these pollutants could be partly retained using filters, and once inside the building they could be eliminated through adsorption and/or diffusion into various materials.

Several approaches have combined simple models that consider neither filtration nor adsorption (Jetter & Whitfield, 2005) with more complex models that consider internal and external filtration, adsorption and desorption onto surfaces, and internal diffusion into materials (Jørgensen et al., 2000). These models can be classified into four categories:

- With neither adsorption nor filtration.
- With filtration and constant adsorption, without desorption.
- With filtration plus variable adsorption/desorption.
- With filtration plus variable adsorption/desorption and internal diffusion.

In the first case, indoor concentration would only be lower than the outdoor concentration by an interval of time equivalent to the inverse of the ventilation frequency. In the other cases, the models find lower concentrations because they take into account adsorption on materials and filtration factors (mainly if the air is recycled) (Casal et al., 1999; Karlsson, 1994; Yuan, 2000). Nevertheless, desorption causes a residual indoor gas concentration over an extended period of time, which causes the indoor concentration to increase and approach the outdoor concentration if the space is not adequately ventilated after the toxic gas plume has passed (Karlsson & Huber, 1996).

All of these models can be represented by a general model based on the one proposed by Shair and Heitner (1974), with the appropriate simplifications applied to each case. Thus, the general mass balance (Fig. 1) can be expressed as follows:

$$\dot{V}\frac{dC_i}{dt} = \dot{V}_o \cdot C_o + \dot{V}_3 \cdot C_o \cdot (1 - f_o) + \dot{V}_2 \cdot C_i \cdot (1 - f_i) - \dot{V}_2 \cdot C_i - \dot{V}_1 C_i - R \cdot C_i + S \cdot C_i \quad (1)$$

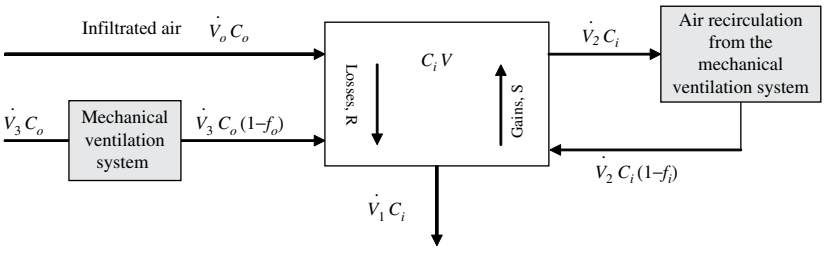

Fig. 1. Schematic diagram of the general ventilation model.