

Determination of ozone reaction probabilities with porous materials

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1 Introduction

Indoor materials can have a large impact on indoor pollutants because of primary emissions, chemical reactions, and associated byproduct formation. We have recently identified promising building materials that remove pollutants and generate little or no harmful byproducts, while requiring no additional building energy inputs. Several examples of these passive removal materials (PRMs), such as activated carbon cloth (ACC) and clay wall coverings, have good ozone scavenging capacity and are of a porous nature. Fundamental removal properties, such as reaction probability, are often difficult to determine for porous materials. This extended abstract outlines a new methodology for determining reaction probability by characterizing pollutant deposition velocity to materials in a plug flow reactor over a range of air speeds.

2 Background

Physical and chemical phenomena related to reactive uptake have typically been modeled as resistances in series (Cano-Ruiz et al., 1993). This theory describes the gas phase removal of a pollutant, or deposition velocity, V_d (m h^{-1}) in terms of the transport limited deposition velocity, V_t (m h^{-1}), a characteristic of the fluid mechanics of a space, and the reaction probability, γ (-), the likelihood of a reaction given a collision between a surface and gas. This relationship is expressed by Equation 1:

$$\frac{1}{V_d} = \frac{1}{V_t} + \frac{4}{\langle V \rangle \gamma} \quad (1)$$

Where $\langle V \rangle$ = Boltzmann velocity, m h^{-1} . Reaction probabilities have been determined by coating materials with a highly reactive substance. This greatly increases γ in Equation 1, and the resulting V_d obtained during such an experiment is approximately equal to V_t .

Knowing V_t allows γ to be calculated for similar experiments where the material is not coated. While this method has been applied with some success (e.g., Morrison and Nazaroff, 2000), recent exploratory experiments by our team have shown this technique may not be applicable to highly porous materials. We hypothesize that coating a porous material reduces overall reaction sites by limiting mass transfer to internal surface area in pores. Therefore, we have investigated the potential for estimating reaction probability from experimental deposition velocities by assuming that the resistance associated with V_t is minimized at elevated airspeeds, in which case Equation 1 simplifies to Equation 2:

$$\frac{1}{V_d} = \frac{4}{\langle V \rangle \gamma} \quad (2)$$

3 Materials and Methods

Thirty experiments were conducted in a galvanized steel duct with a cross-sectional area 0.023 m^2 and length of 7.7 m, designed to act as a turbulent plug flow reactor. A variable speed fan was used to provide air flow at speeds ranging from 0.21 to 3.91 m s^{-1} . Target inlet ozone concentrations were 100 ppb and generally ranged from 80-120 ppb. Steady-state ozone deposition velocities to three building materials (stainless steel, activated carbon cloth (ACC), perlite-based ceiling tile) were calculated from inlet and outlet ozone concentrations, measured using UV absorption spectroscopy.

Experimental data were fit to a logistic function with non-linear regression to determine “saturation” deposition velocities associated with a specific material under conditions of high mass transport. Reaction probability was determined by inserting this saturation deposition velocity for V_d in Equation 2

3 Results

Figure 1 illustrates the relationship between ozone deposition velocity and increases in bulk airspeed for ACC and compares the relationship to theoretical estimates of transport-limited deposition velocity from mass transfer theory (Sparks et al., 1996). Deposition velocity values shown in Figure 1 have been corrected for background losses to the stainless steel flow chamber. Equation 2 produces a reaction probability on the order of 10^{-4} . Grontoft (2002) determined reaction probabilities of ozone to ACC on the order of 10^{-5} in a similar manner but over a narrower range of low Reynolds number flow conditions (bulk airspeeds ranging from 0.00075 to 0.0025 m s^{-1}).

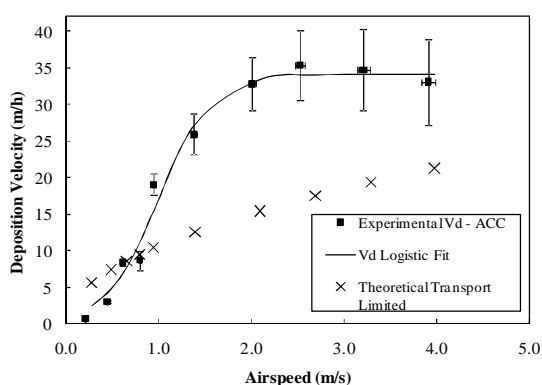


Figure 1. Experimental deposition velocity to activated carbon cloth measured during experiments at elevated airspeeds compared to theoretical determinations of transport-limited deposition velocities.

ACC has a large surface area and high porosity. Past research has identified high deposition velocities to this material, particularly at elevated airspeeds. Materials with high deposition velocity may be well suited for this method due to the large difference between inlet and outlet ozone concentrations. However, uncertainty resulting from transport through pores at high airspeeds as well as an unknown effective material surface area complicate determination of reaction probability. Other tested materials (not shown for brevity) also introduce the possibility of depletion of material reaction sites, resulting in reduced observed ozone deposition velocity for experiments conducted under similar conditions.

As Figure 1 shows, theoretical estimates of transport-limited deposition velocity are significantly lower than experimental

measurements of ozone deposition velocity. If the assumption of negligible transport resistance were not made, combining this theory and experimentation would result in negative estimations of reaction probability. Two related phenomena may be important actors in these removal processes that receive limited attention in indoor environmental literature: 1) incorporation of surface area effects which prohibit the application of existing models of mass transfer theory and 2) diffusion and advection through pores which may limit the rate of ozone removal at elevated airspeeds.

4 Conclusions

A new method to determine ozone reaction is presented. Comparison of experimental data with mass transfer theory results in consistent underestimates of modeled transport-limited deposition velocities. Future work will begin to develop empirical and mechanistic models of ozone transport into porous materials by characterizing penetration depths and breakthrough times associated with horizontal flow over porous materials.

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5 References

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