

Combined air, heat, moisture and VOC transport in whole buildings

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ABSTRACT

Thermal and moisture performances of whole buildings are rather well understood today and various models exist for simulating those. However, models for calculating VOC emissions from or through building envelope parts are still rare and often need specific material properties for each transported compound. A comprehensive model for indoor air quality should be able to account for the coupling of thermal, moisture, air and VOC processes and make use of generalized material properties.

In this paper, we first present a computer simulation model for predicting the combined air, heat, moisture and pollutant transport, followed by a discussion on the material properties required for the model simulation, and then present the predicted and measured results for individual materials and a typical wall assembly of residential houses with the objective of demonstrating the usefulness of the simulation model.

INDEX TERMS

Modelling; VOC; Moisture; Mass transfer; Air infiltration

INTRODUCTION

Indoor air quality (IAQ) ventilation and building envelope components are interconnected. The sources and transport mechanisms of VOCs and contaminants in indoor air need to be understood and estimated when designing healthy buildings. Emissions from building materials are commonly taken only from surface materials when estimating the effects of building structures on indoor air quality. Surface materials are, however, just a part of the contaminant sources in the indoor environment. Envelope structures as a whole and the materials in various layers of the structures can be even more significant factors affecting the indoor air quality than surface materials. The extent to which these emissions affect indoor air quality depends on the performance of the building structure as a system, i.e. if the emissions are transported inwards or outwards by diffusion and convection airflows. Suitable temperature and humidity are often a prerequisite for the development of detrimental effects (e.g. mould growth, rot, material decay) in building materials.

In order to predict the effects of the whole building structure on IAQ under intended load and environmental conditions, it is necessary to understand the combined air, heat, moisture and pollutant transport in the building structures as well as the generation of VOCs from individual material layers. The predictions will help develop better designs of building envelope assemblies and HVAC systems to control the leakage flow paths and rates, moisture content in the materials and the transport of VOCs into the building. The transport model developed will also be useful for understanding how much protection the building envelope can provide against airborne chemical or biological agents (CBA) in case of internal or external CBA releases. The building envelope model equations can further be implemented in whole building simulation models once the modelling of building details has been validated.

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DEVELOPMENT OF A NOVEL NUMERICAL MODEL

The sorption and transport of VOCs and moisture in porous materials can be simulated using the same equations. Each VOC would just require its own transport properties for each material. The number of different VOCs is too large to make it feasible to measure all the VOC transport properties for all the materials, and for all the VOCs we are interested in. For this reason, this paper investigates the similarities in moisture modelling with VOC modelling. The material properties for various VOCs for the same material and how they could be estimated without measured data for the individual compound is presented.

Moisture may affect the VOC sorption, transport and source. Water and VOCs share the same pore volume when adsorbed in porous materials and variations in moisture contents in materials may change the emission rates by changing the sorption phenomena. However, these effects need more investigation and will be discussed in the future papers. At present, the model is used without considering the effects of moisture on the VOC processes.

It is important to make a difference between the different types of sources for emissions and how they behave in the whole system. The so-called primary and secondary sources have their differences in the origin of VOCs. Primary sources are based on off gassing of initial VOC content after manufacturing; secondary sources are created during the life of the material in its intended use. The secondary source may be generated and initiated by excess moisture (reactions, mould growth, etc.). Modelling of emission sources is a research area that needs more attention and is not discussed here.

MODEL EQUATIONS

A numerical model for heat, air and moisture transport was modified and the model equations for calculating emission transport and storage/sorption were added. The same format of equations was used for both VOC and the moisture transport equations. In what follows, we present the similarities of the model equations for both moisture and VOC calculations.

Sorption

Moisture storage/sorption capacity of porous materials can be described by the following equation:

$$u = f(RH, T) = f(RC, T) \quad (1)$$

where u = moisture (or VOC) content [kg-water/kg-dry material]; $RH = P_v/P_{v,sat}(T)$, RH (or RC = relative concentration) [–]; and T = temperature [K]. The storage capacity of VOCs in porous materials for a given temperature under low VOC concentration conditions is often presented with the partition coefficient:

$$K_{ma} = C_m / C_a \quad (2)$$

where C_a = the VOC concentration in air at the air–material interface [kg/m³] and C_m = the VOC content in the porous material at the air–material interface [kg/m³]. Note that

$$u_{VOC} = C_m / \rho_0 = K_{ma} C_a / \rho_0 = K_{ma} C_{a,sat} RC / \rho_0 = K_{ma} P_{v,sat} M \cdot RC / (\rho_0 RT) \quad (3)$$

where ρ_0 is the material's density [kg/m³], $C_{a,sat}$ = saturated VOC concentration for the given temperature and M = molecular weight [kg/mol].

Transport by Diffusion and Airflow

The commonly used equations for diffusion of water vapour are based on either vapour pressure or pore air concentration

$$q_{m,vapour} = -\delta_p \nabla P_v + \rho_{dry\ air} \vec{v} C_a \text{ or } q_{m,vapour} = -D \nabla C_a + \rho_{dry\ air} \vec{v} C_a \quad (4)$$

where δ_p = vapour permeability [kg/msPa], v = velocity [m/s] and D = effective moisture diffusivity [m^2/s]. Liquid flow for VOCs can be assumed to be negligible at the concentration levels typically found for these compounds in porous materials.

Mass Balance Equation

After conversions from different forms of equations the final equations to solve either moisture or VOC transport and storage will look the same. Finally, we get

$$\rho_0 \frac{\partial u}{\partial t} = -\nabla \cdot q_{m,vl} - \nabla \cdot q_{m,air} + S \quad (5)$$

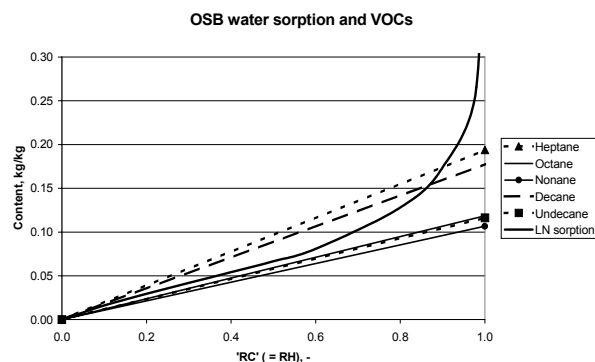
where S = source [kg/m^3s].

MATERIAL PROPERTIES FOR MODELLING

In order to use the VOC prediction model described above, it is essential to have accurate and reliable model parameters including the diffusion coefficient, D_{voc} , partition coefficient, K_{ma} and initial concentrations in the materials. There have been several methods developed for determining these parameters using small environmental chambers (An *et al.*, 1999; Bodalal *et al.*, 1999; Zhang *et al.*, 2002). Based on these limited VOC data and the more abundant existing data on moisture transport properties, the analogy between VOC and moisture transport is explained, and the possibility of developing correlations between VOC and moisture transport properties of building materials is investigated.

Sorption Properties

If the equation describing sorption of VOCs is presented in the same way as the sorption curve for moisture in porous materials, it becomes evident that these isotherm curves indeed look very similar and that the same sorption curve might be used as the first guess for different gaseous components for the sorption/desorption phenomenon. For example, Figure 1 shows the sorption curve for water vapour and various other gaseous components in OSB.



VOC	K_{ma} (-)	Diffusion coefficient, D_m (m^2/s)	$D_{mg} = D_m \times K_{ma}$ (m^2/s)
Heptane	472	2.34e-10	1.11e-07
Octane	998	1.12e-10	1.12e-07
Nonane	2369	4.51e-11	1.07e-07
Decane	12028	1.07e-11	1.29e-07
Undecane	25932	7.24e-12	1.88e-07

Figure 1 Sorption curves of OSB for water vapour (LN) and selected VOCs (extrapolated) are shown on the left as a function of RH/concentration. Diffusion coefficients in OSB when the potential is either total concentration C_m or the concentration in the pore space air C_a (D_m and K_{ma} from: Bodalal *et al.*, 1999) are presented on the right.

The RH of water vapour in outdoor and indoor air typically covers the whole range of RH whereas the VOC content (relative to saturation) in air is usually very low. This means that the sorption phenomena may be slightly different at typical conditions for moisture and

VOCs. Sorption isotherm curves for VOCs at high concentrations are not yet well known. These material dependent VOC retention properties become important when we investigate the primary sources from porous materials or when we have a high initial concentration of a VOC in the pores of the material.

Diffusion Coefficients

The diffusion coefficient (or vapour permeability) for VOC transport in the presented model is based on the vapour concentration (or vapour pressure) in the pore air as the potential. The coefficient may depend on temperature, humidity and the VOC concentration. At this stage of investigating the properties we can assume that the VOC concentration does not affect the diffusion coefficient. The concentration of VOCs in the pore air will depend strongly on the local temperature via the temperature dependent saturation vapour pressure.

Examples of diffusivity in gas phase D_{ma} for some VOCs in oriented strand board (OSB) have been calculated and are shown in Figure 1. Water vapour permeability below 50% RH in OSB is according to values found in the literature: approximately $0.3\text{--}1.0 \times 10^{-12}$ kg/ms Pa that is equal to approximately $0.4\text{--}1.4 \times 10^{-7}$ m²/s when vapour concentration is used as the potential. Diffusivities for various gaseous components in air under the standard atmospheric condition can be represented within reasonable accuracy by a simple curve fit (Figure 2). For this limited data, water vapour diffusivity and the diffusivity for various VOCs seem to be reasonably at the same level in the same material. However, in Figure 1 the VOC diffusivity in the material seems to increase as molecular weight increases whereas in air the diffusion coefficients of VOCs decrease as the molecular weight increases (Figure 2, left).

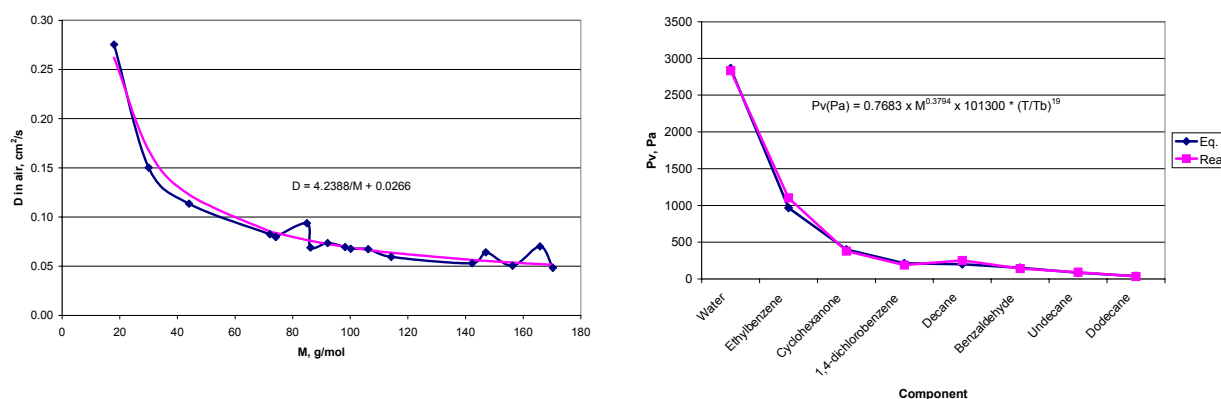


Figure 2 Diffusivity of VOCs in air is estimated as a function of molecular weight on the left. Symbols are for quantities that are measured or calculated with equations from the literature for single VOCs, line without symbols is a curve fit estimation through the presented values.

On the right, the saturation vapour pressure is given as a function of the compound's molecular weight M [g/mol] and boiling point temperature T_b [K] at 23°C obtained from the literature.

Saturation Vapour Pressures of VOCs and Water Vapour in Air

Saturation vapour pressure of water vapour as well as that of VOCs is a strong function of temperature. The saturation vapour pressure is an important parameter in moisture and VOC transport calculations, since the pore space air concentration depends heavily on the temperature and since the pore space air concentration (or vapour pressure) is the main driving force for vapour diffusion. The total concentration of VOC or water vapour in the porous material is related to the pore space air concentration via the sorption curve. The changes in local temperature affect the pore air vapour concentration via the temperature dependence of the saturation vapour pressure.

The saturation vapour pressure of gases in air can be found to correlate with the boiling point temperature and the molecular weight. Information about the gas properties is not

always readily available for the many VOCs. A generic equation was formed for estimation purposes. Water vapour and a selection of eight VOCs and their saturation vapour pressures were curve fitted and a simple correlation was developed as a function of molecular weight and boiling point temperature (Figure 2, right). The maximum error was 25%.

EMISSIONS FROM INDIVIDUAL MATERIALS

The model equations were tested against measurements for single materials in a small chamber. The emission rates of α -pinene and 2-pentyl furan from an OSB-board were investigated (Zhang *et al.*, 1999) and are shown here. Material properties for the calculation of VOC transport in OSB were calculated by taking the moisture properties and by multiplying the moisture diffusivity with the ratio of the VOC diffusion coefficient in air to water vapour diffusion in air. The saturation vapour pressure was calculated with an equation based on the molecular weight and boiling point temperature (Figure 2, right). The simulated and measured concentrations in the chamber air are in good agreement (Figure 3, left).

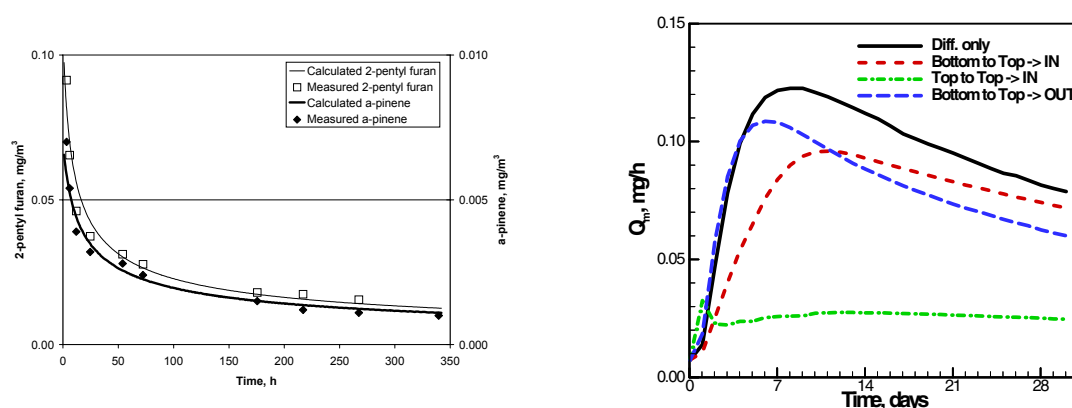


Figure 3 Left: small chamber test results for measured and calculated VOC concentrations in the chamber air as a function of time for OSB. On the right are the emission rates of 2-pentyl furan from a full wall (1 m wide) to the outdoor and indoor air with various air infiltration patterns (with vapour retarder) or with no air infiltration and with permeable building paper.

EMISSIONS FROM A WHOLE BUILDING STRUCTURE

To date well-controlled measurements of emissions from whole building structures do not exist to validate the model equations in their natural environment with heat, air and moisture storage and transport processes affecting the processes in multi-layered structures. Such experimental data will become available in the near future with the construction of the new indoor/outdoor environmental chamber at Syracuse University (Herrman *et al.*, 2002).

The simulated predictions of emissions from OSB and the fraction of the total emissions that end up in the indoor air are presented with different air infiltration patterns through a light-weight wall structure (material layers: vinyl siding, OSB, mineral wool insulation, polyethylene vapour barrier, gypsum board). The air leakage paths were assumed to be located close to the bottom of the wall on the exterior side and to the top of the wall on the interior side. The air would flow through the insulation layer from outside to inside. The airflow rate was selected to be such that the airflow through the wall would account for approximately 0.115 ach in a square house with floor area of 10 m \times 10 m. Calculations were carried out under a constant temperature of 23°C. The initial concentration of other layers was zero except for OSB.

The simulated emission rates of 2-pentyl furan are presented in Figure 3. The effect of infiltrating air on the emission rates to the indoor air is evident. After a period of 2 weeks from the beginning, the air infiltration was found to convectively transport almost as much VOCs to the indoor air as that which is diffused to the outdoor air.

CONCLUSIONS

The new computer simulation model for predicting the combined air, heat, moisture and pollutant transport has been used for simulating emission rates from individual materials, layered material combinations and from a whole building wall. The predicted and measured results were in relatively good agreement with each other. The analysis of the transport and storage properties of moisture and VOCs in porous materials revealed that it could be possible to use the same material properties for gaseous components other than water vapour with some modifications based on the basic properties of the gas. Well-defined, small and full-scale laboratory experiments are needed to benchmark and validate the model predictions. These series of test cases will be carried out in the near future. If these comparisons are successful the model equations can readily be used in whole building simulation environments.

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