MODELLING CONTAMINANT TRANSPORT IN ENCLOSED SPACES - A STATE-SPACE APPROACH

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Abstract. Multizone modelling is a standard tool in the study of contaminant transport within enclosed spaces. This work considers an alternative state-space approach to the calculation of contaminant transport under constant flow conditions. An analytical solution is expressed for the concentration dynamics for constant release conditions. This provides an opportunity to avoid the numerical integration normally required by standard approaches. Insight into the late decay phase is gained by consideration of the eigenvectors and eigenvalues of the state matrix. An example building is considered and the state-space approach used to calculate the concentration dynamics. The decay rate in the late decay phase is compared with the nominal air change rate for a wider range of buildings and seen to show strong correlation with these measures falling within a factor of two for most buildings. Steady state concentrations resulting from continuous releases within a building are addressed using a simple matrix calculation and visualisation. The state-space approach shows considerable promise for rapidly assessing contaminant transport in enclosed spaces.

1. Introduction

There is a need to understand how airborne chemical, biological and radiological materials move through indoor spaces so that the impact of terrorist attacks within or close to buildings can be assessed. People spend much of their time indoors, so occupant densities and residence times can be high. Enclosed spaces also reduce the dilution of airborne material resulting in higher concentrations for longer periods when compared to the outdoors. Exposure of building occupants depends on the details of the scenario and the building. Understanding contaminant transport and the resulting exposure is a prerequisite for improving security and resilience.

There are a number of ways to tackle these problems using experimental measurements and numerical modelling and the best choice depends on the scenario in question. Multizone modelling is one commonly used numerical approach that lends itself to whole building studies [10, 4]. It treats spaces within the building as a series of discrete interconnected volumes and uses a two-step process to predict contaminant transport. Firstly the air flow into and through the building is predicted. Secondly these flows are used to calculate the dispersion of contaminants. Existing models such as CONTAMW [14] and COMIS [2] use numerical integration to perform this second step. For large studies this can become a time consuming part of the process.

This paper describes an alternative method of calculating this contaminant dispersion step. The governing system of ordinary differential equations have been recast using a state-space formulation. This makes clear the strong parallels with other application areas where dynamic systems are important such as transport of metabolites in biomedical models [3], ecological models [13], control theory [1] and electrical systems [5]. This approach develops earlier work for building studies by

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Sinden [9] and Sandberg [8]. Using this form, the time dependent concentration solution can be expressed in terms of the matrix exponential. When the controlling matrix is diagonalisable it is possible to write down an analytical expression, in terms of the eigenvalues and eigenvectors, for the concentration at any time without the need for integration. The integrated exposure can also be expressed analytically. In addition, key features of the concentration dynamics, such as the long term decay rate and the concentration ratio, emerge from the eigensystem analysis. Finally, it is possible to rapidly analyse the response of one or more buildings to continuous contaminant releases. Parts of this analysis have recently been summarised in [6].

This alternative approach provides an increase in speed that makes it practical to analyse a wide range of scenarios for applications such as optimising detector or sampler placement [11] or estimating source terms based on detector response [12]. The eigenvalues and eigenvectors also provide crucial insight into the dynamic system behaviour that is independent of specific scenarios.

2. Theory

2.1. **Assumptions.** A multizone system is assumed, where each zone has a fixed volume of air and is connected through at least one link to the whole system and each zone is instantaneously well-mixed. It is assumed that the air flows into and out of the system and between zones are constant, and are known in advance. It is assumed that contaminant concentrations are dilute such that they do not affect the air density and that there are no non-linear effects due to high concentrations.

2.2. **State-space formulation.** Consider a system of n interconnected zones. The rate of change of concentration for each of the zones, $\dot{\mathbf{x}}$, can be written in state space notations as:

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \tag{1}$$

The matrix $\mathbf{A}$ controls the system dynamics based on the current system concentration state $\mathbf{x}$. For this application $\mathbf{A}$ is defined as:

$$\mathbf{A} = \mathbf{V^{-1}}\mathbf{Q} \tag{2}$$

where $\mathbf{V}$ is a diagonal matrix with $V_{i,i} = V_i$ where V_i is the volume of zone i in [m^3] and $V_{i,j} = 0$ for $i \neq j$.

$$\mathbf{Q} = \begin{bmatrix} -Q_{1,1} & Q_{1,2} & \cdots & Q_{1,n} \\ Q_{2,1} & -Q_{2,2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & Q_{n-1,n} \\ Q_{n,1} & \cdots & Q_{n,n-1} & -Q_{n,n} \end{bmatrix} \tag{3}$$

where $Q_{i,j}$ is the flow into zone i from zone j when $i \neq j$ and $Q_{j,j} = (-\sum_{i=1}^{n} Q_{i,j} - Q_{0,j})$ is the flow out of zone j, where $Q_{0,j}$ is the flow of air out of the system from zone j. All flow rates have units of [m^3 s^{-1}].

The term $\mathbf{Bu}$ accounts for the input of contaminants into the system, with $\mathbf{B} = \mathbf{V^{-1}}$. The input $\mathbf{u}$ includes both the flow of airborne contaminants into the building from the exterior and releases within the zones of the building. A full definition of these terms and the representation of losses within the building is given in [6].

2.3. **Solution.** The use of the state-space formulation allows some of the system behaviour to be readily determined. The following results provide useful information without the need to resort to a full numerical analysis.

2.3.1. *Concentration dynamics.* A solution to equation (1) can be written as follows:

$$\mathbf{x}(t) = e^{\mathbf{A}(t-\tau)}\mathbf{x}(\tau) + \int_{\tau}^{t} e^{\mathbf{A}(t-\mu)}\mathbf{B}(\mu)\mathbf{u}(\mu)d\mu \tag{4}$$

where t is the current time, τ is the time at the start of the release and μ is a variable of integration. When the state transition matrix $\mathbf{A}$ is diagonalisable then (4) can be expressed as:

$$\mathbf{x}(t) = \mathbf{S}e^{\mathbf{\Lambda}(t-\tau)}\mathbf{S^{-1}}\mathbf{x}(\tau) + \int_{\tau}^{t} \mathbf{S}e^{\mathbf{\Lambda}(t-\mu)}\mathbf{S^{-1}}\mathbf{B}(\mu)\mathbf{u}(\mu)d\mu \tag{5}$$

where $\mathbf{\Lambda}$ is an n by n matrix with the eigenvalues arranged on the diagonal ($\mathbf{\Lambda}_{i,i} = \lambda_i$). $\mathbf{S}$ is a matrix containing the right eigenvectors associated with each eigenvalue arranged as columns.

In general the zone volumes, and therefore $\mathbf{B}$, will be time-invariant. When $\mathbf{u}$ is constant over the integration period (for example for a uniform release rate or a constant external concentration):

$$\mathbf{x}(t) = \mathbf{S}e^{\mathbf{\Lambda}(t-\tau)}\mathbf{S^{-1}}\mathbf{x}(\tau) - \mathbf{S}\mathbf{\Lambda}^{-1}\Big(\mathbf{I} - e^{\mathbf{\Lambda}(t-\tau)}\Big)\mathbf{S^{-1}}\mathbf{B}\mathbf{u} \tag{6}$$

where $\mathbf{I}$ is an n by n identity matrix. This expression gives an analytical solution to the time-dependent concentration in a multizone system subject to initial conditions and constant inputs.

2.3.2. *Decay phase concentrations.* When there are no inputs into the system $\mathbf{u} = 0$ and the concentration dynamics for a diagonalisable case are given by:

$$\mathbf{x}(t) = \mathbf{S}e^{\mathbf{\Lambda}(t-\tau)}\mathbf{S^{-1}}\mathbf{x}(\tau) \tag{7}$$

As t becomes large the rate of decay for each concentration tends to a constant value, given by the eigenvalue of smallest magnitude. The concentrations then maintain a constant ratio to each other given by the associated eigenvector. For further details see [6].

2.3.3. *Steady state concentrations.* It is also interesting to examine the distribution of concentrations throughout a multizone building at steady state when there is a constant input into the system. At steady state $\dot{\mathbf{x}} = 0$ and substituting into (1) and rearranging gives an expression for the steady state concentration vector for any $\mathbf{u}$:

$$\mathbf{x} = -\mathbf{A}^{-1}\mathbf{B}\mathbf{u} \tag{8}$$

This provides a useful mechanism for calculating the steady state concentration distribution provided that $\mathbf{A}^{-1}$ exists.

3. Example applications

3.1. **Nine zone building.** To illustrate the benefits of this alternative approach we first consider an example mechanically ventilated building. The three-floor building is divided into nine zones as shown in Figure 1. If we consider the case where there is a constant release rate of contaminants in Floor 1 for 1 h then we can use (6) to calculate the concentration dynamics in each zone in the building. Figure 2 shows the result. It can be seen that the concentration rises rapidly in each zone during the period of release before the concentrations begin to decay. It is interesting to note that the concentrations cross over. Eventually the decay rate

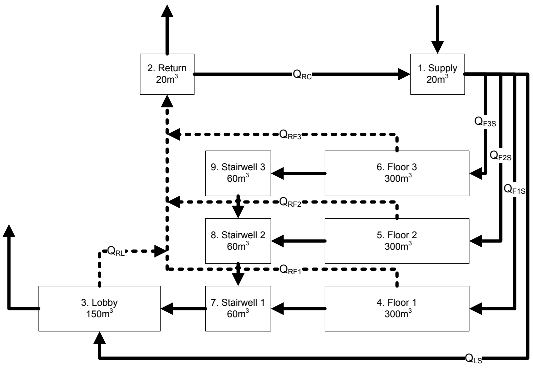


FIGURE 1. Diagram of nine zone mechanically ventilated building.

reaches a constant value as shown by the constant gradient on the logarithmic plot. During this phase the concentrations are different but maintain a constant ratio to each other as discussed in 2.3.2.

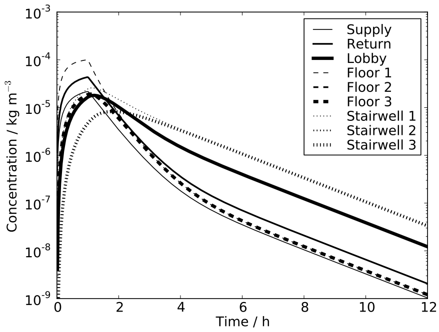


FIGURE 2. Predicted concentrations against time for a release on floor 1 in a conceptual nine-zone building.

3.2. **Long term ventilation rate.** A common approach to assessing the decay rate for contaminant in a building is to consider the building as a single well-mixed space. In this case the decay rate is given by the nominal air change rate defined as the total fresh air flow rate divided by the total interior volume. As discussed in Section 2.3.2, for a multizone building the smallest magnitude eigenvalue will determine this decay rate.

A large number of multizone models of a range of US residential buildings have been published by NIST [7]. These models were converted from CONTAMW models into a state-space representation and the air change rate and eigenvalues calculated. The resulting values are plotted in Figure 3 and it can be seen that there is a strong correlation between these two ventilation measures, with most examples falling within a factor of two of each other. In general the detached houses appear to have a smaller eigenvalue than the air change rate. This is believed to be due to the presence of a poorly ventilated crawlspace below the ground floor in these models that acts as a reservoir and reduces the decay rate in the later decay phase.

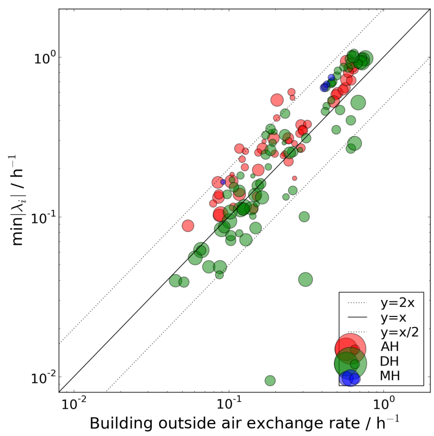
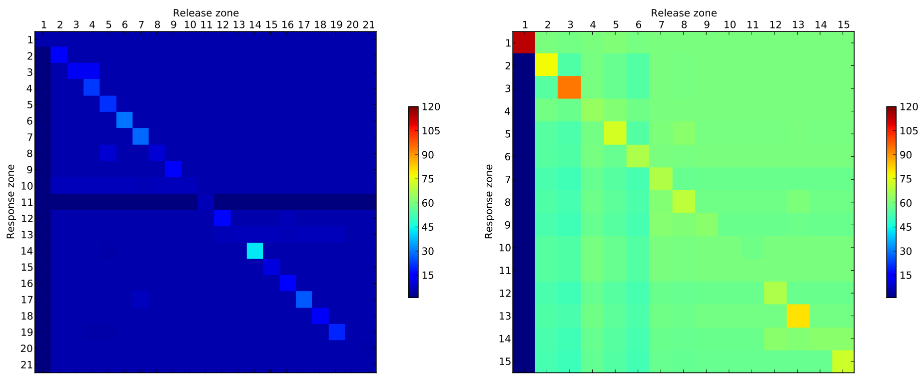


FIGURE 3. Minimum magnitude eigenvalue versus nominal air change rate for modelled US residential buildings. AH = attached houses, DH = detached houses and MH = manufactured houses.

3.3. **Steady state concentrations.** The same model buildings described in Section 3.2 were used to consider the impact of the location of a single constant source of contaminant within the building. A release rate of 1 mg s^{-1} was applied to each zone in turn using (8). The resulting concentrations are shown in Figure 4 (A) and (B). Each column represents the concentrations resulting from a continuous source within that zone.



(A) (B)

FIGURE 4. Steady state concentration response matrices for two detached houses from [7] with 21 zones (A) and 15 zones (B). Steady state concentration in each zone indexed by row for a constant release rate in the zone indexed by column. Colour bar shows concentration in units of mg m^{-3} for a release rate of 1 mg s^{-1}.

The figures show a clear difference in the response to the releases between the two buildings. Figure 4 (A) shows lower concentrations than in (B). This is a result of higher ventilation rates in (A) than in (B). The diagonal entries show higher values than the off-diagonal entries since the concentration will be highest in the zone where the release is located. A single plot can be used to represent a large number of these visual representations of a building's response to contaminant sources. In this way it is possible to rapidly assess the potential impact on a large number of buildings. In this example no consideration is given to removal mechanisms such as filtration and deposition of contaminants. However, the full formulation described in [6] allows these to be incorporated into the matrix **A**.

4. Summary and conclusions

Expressing the key equations for contaminant transport in multizone buildings in a state-space form makes it straightforward to analyse the behaviour of the system. For diagonalisable matrices the long term decay behaviour is given by the eigenvalues and eigenvectors. This decay behaviour is seen to be close to, but different from, the whole building nominal air change rate for a group of residential model buildings. The state space form also provides a simple way to assess the concentrations likely to arise from continuous contaminant releases in different locations. In addition to the features drawn out here, there are a number of other possible calculations that can be performed directly, including the cumulative exposure of building occupants [6].

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