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Implementing state-space methods for multizone contaminant transport

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ABSTRACT

The "well-mixed zone" approximation is a useful model for simulating contaminant transport in buildings. Multizone software tools such as CONTAM [1] and COMIS [2] use time-marching numerical methods to solve the resulting ordinary differential equations. By contrast, the state-space approach solves the same equations analytically [3]. A direct analytical solution, using the matrix exponential, is computationally attractive for certain applications, for example, when the airflows do not change for relatively long periods. However, for large systems, even the matrix exponential requires numerical estimation. This paper evaluates two methods for finding the matrix exponential: eigenvalue decomposition, and the Padé algorithm. In addition, it considers a variation optimised for sparse matrices, and compares against a reference backward Euler time-marching scheme.

The state-space solutions can run several orders of magnitude faster than the reference method, with more significant speedups for a greater number of zones. This makes them especially valuable for applications where rapid calculation of concentration and exposure under constant air flow conditions are needed, such as real-time forecasting or monitoring of indoor contaminants. For most models, all three methods have low errors (magnitude of median fractional bias $<3\cdot10^{-5}$, normalised mean square error $<3\cdot10^{-7}$, and scaled absolute error $<4\cdot10^{-4}$). However, for the largest model considered (1701 zones) eigenvalue decomposition showed a dramatic increase in error.

1. Introduction

1.1. Motivation

In certain applications, the time needed to run a multizone model of pollutant transport in a building becomes a significant aspect of the modelling effort. Inverse problems, in particular—for example, locating a contaminant source based on sensor measurements [4], or finding best-fit model parameters based on experimental data [5]—may require hundreds or even thousands of model runs. Similarly, optimisation studies typically require hundreds of simulations [6]. In addition to the sheer number of runs, for a sufficiently complicated building, or when simulating long periods of time, each run of a multizone model may take on the order of minutes. Modelling fast transport processes such as chemical reactions, sorption, or high air flow rates exacerbates the problem, by forcing a time-marching numerical solver to use short time steps in order to control the solution accuracy [7].

As an alternative to time-marching schemes, direct analytical solution of the transport equations has the potential to be faster, especially in cases where air flow remains constant for long periods [3]. This paper explores several implementations of the state-space approach to contaminant transport in multizone building models. It introduces the relevant theory, proposes a number of solution strategies, then compares their accuracy and speed using existing multizone building models.

1.2. Background

Contaminant concentrations in buildings and other enclosed spaces can be predicted using a range of approaches from simple single zone models [8] to high-fidelity computational fluid dynamics methods (CFD) [9]. Single zone models cannot predict the spatial distribution of airborne contaminants within a building, although they may play a role in rapid calculations for emergency planning [10]. CFD methods, on the other hand, can provide a great deal of information on the spatial and temporal behaviour of

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contaminants. However, CFD requires a large amount of information to specify the geometry and boundary conditions of the space. It is also computationally intensive, to the point that whole-building CFD remains impractical. Arguably the specificity of the approach limits the applicability of the results from one simulation to other cases.

Multizone models, such as CONTAM [1] and COMIS [2], provide an intermediate level of detail. They predict air flows and contaminant concentrations through whole buildings. This approach has been widely used for a range of applications including the transport of VOCs and CO_2 [11], environmental tobacco smoke [12] and infectious diseases [13], air monitoring [14] and ventilation studies in tall buildings [15–18]. The multizone approach has also been extended by the introduction of sub-zones [19]. A useful review of multizone modelling and a comparison with other methods can be found in Refs. [20,21].

Briefly, multizone models find the steady-state air flows between building zones, including rooms and ventilation system components, and the outdoors [22]. These flows then drive the transport of contaminants. Here, the flows are considered fixed over the course of each transport time step. However, they may change between time steps, for example due to changes in zone temperatures, wind, or mechanical ventilation.

The transport system assumes the flows carry contaminants between well-mixed zones, in which the contaminant mixes instantaneously and perfectly. The transport model also can include pollutant sources and sinks, including losses due to filtration and deposition. This leads to a coupled set of ordinary differential equations that describe the time rate of change of contaminant concentration or mass in each zone [23,7]. Typically these equations are linear in the unknown concentrations.

Recently state-space methods have been used to study particle behaviour in indoor environments [24] and to solve the transport system for CFD [25] and multizone air flow solutions [3]. This formulation provides insight into the concentration dynamics, and allows closed-form solutions to the governing equations.

State-space solutions involve finding matrix exponential terms. This paper evaluates three calculation methods; eigenvalue decomposition, the Padé method and a Krylov subspace method. Eigenvalue decomposition replaces the matrix with a product of three matrices; the eigenvector matrix, a diagonal matrix composed of the eigenvalues and the inverse of the eigenvector matrix [26]. The Padé method scales the matrix to reduce the norm to order 1, computes the Padé approximant to the matrix exponential, and then squares the resulting matrix to undo the scaling [27]. The Krylov subspace method is optimised for sparse matrices, and uses a reduced matrix together with the Padé method to calculate the matrix exponential [39]. Details of these approaches are laid out in the theory section that follows.

The numerical solutions of air flow and concentration dynamics within multizone models have been studied previously [22,7,1] and methods for solving the matrix exponential for general use have been outlined by a number of authors [28,27,29]. However, this work explores the accuracy and speed of direct solution methods for multizone state-space concentration dynamics for the first time.

2. Theory

2.1. State-space formulation

The state-space method as applied to the multizone transport problem is described in Refs. [23,3]. The key elements are repeated here in order to explore the form of the concentration and exposure solutions. The concentration within any zone is defined as x_i [kg m^{-3}], where i is the zone index. The concentrations over the whole building are given by $\mathbf{x}$, a column vector of length n, where n is the number of zones in the multizone model. The rate of change of $\mathbf{x}$ is given by

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

where the vector $\mathbf{Bu}$ describes the rate of input of contaminants into the system, for example due to sources within the building, or due to inflows from nodes, like the outdoors, with a known concentration. Each entry in the vector defines the source of contaminants [kg m^{-3} s^{-1}] in the corresponding zone [3].

The state matrix $\mathbf{A}$ accounts for the transfer of contaminants between zones, and the removal of contaminants through ventilation and other mechanisms, such as deposition and filtration. In the case where there are no removal mechanisms other than direct ventilation, $\mathbf{A}$ is given by

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

where $\mathbf{V}$ is a diagonal matrix whose entries $\mathbf{V}_{i,i} = V_i$, where V_i is the volume of the ith zone. $\mathbf{Q}$ is an n by n matrix describing the flows between and out of the zones. The flow into zone i from zone j is $Q_{i,j}$ when $i \neq j$. $Q_{i,i} = -(\sum_{j=1(j\neq i)}^{n} Q_{j,i} + Q_{0,i})$ is the flow out of zone i, where $Q_{0,i}$ is the flow of air out of the system from zone i. All flow rates have volumetric units of [m^3 s^{-1}]. The more general case where there are removal mechanisms is accommodated by modifying $\mathbf{A}$, as described in Ref. [3]. Note that in practice, since the air flows come from a mass balance, they may be specified in [kg s^{-1}], in which case the concentrations are predicted on a mass fraction basis, e.g., [kg kg^{-1}], accordingly. Since the off-diagonal elements of the matrix $\mathbf{A}$ represent the flows between zones, matrices of increasing size will be increasingly sparse since each zone will have a limited number of connecting zones. Reference [3] includes an example matrix for a nine zone building which illustrates the structure of the matrix.

2.2. Time-marching solution

Multizone software programmes solve the transport system by discretising (1) over time. To advance from time t_n to t_{n+1}, the discretisation relates $\mathbf{x}(t_{n+1})$ to $\mathbf{x}(t_n)$, and to the rates of change $\dot{\mathbf{x}}$ at those times [30]. As these time-marching algorithms advance through simulated time, their error depends primarily on: (1) the step length $h = t_{n+1} - t_n$, with shorter steps generally providing lower errors; and (2) the details of the discretisation, with higher-order polynomial fits to values and derivatives at earlier times t_{n-1}, t_{n-2}, and so on, generally providing lower errors.

The simplest time-marching scheme, forward Euler, projects the rate of change calculated at t_n forward over the entire step. Implicit methods, such as backward Euler, define a system of algebraic equations that must be solved for $\mathbf{x}(t_{n+1})$. While computationally more costly, implicit methods have better stability than explicit methods. Applied to whole-building transport problems, stable methods converge to the correct steady-state concentrations, even if the time steps are too long to make accurate transient predictions [30]. CONTAM v 3.1 uses backward Euler as its default solver [1], although it also provides higher-order methods [7].

Backward Euler sets

$$\mathbf{x}(t+h) = \mathbf{x}(t) + h\dot{\mathbf{x}}(t+h). \tag{3}$$

In the state-space form substituting with (1) gives

$$\mathbf{x}(t+h) = \mathbf{x}(t) + h\mathbf{A}\mathbf{x}(t+h) + h\mathbf{B}\mathbf{u}, \tag{4}$$

where $\mathbf{Bu}$ is assumed constant over the time step. Rearranging gives