Reduced-order ventilation models for the prediction of indoor pollutant dispersion

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Abstract. This work introduces the development of reduced-order ventilation models for transient pollutant dispersion. We focus on transients resulting from a step change in pollutant source distributions, and we further simplify this to a decay problem. The solution to this is formulated in terms of a matrix exponential, that is accurately represented with only a few dominant eigenmodes. Using a 2D ventilation case, dominant eigenmodes with their physical relevance, and pollutant concentration results are presented. We find that the first 4 eigenmodes are sufficient to predict the pollutant concentration decay throughout the ventilation enclosure. We also find that the complex eigenmodes play an important role in the indoor recirculation processes.

Keywords: ventilation, CFD, CO\(_2\) decay, reduced-order models, eigenmodes

1 Introduction

In real life, mechanical ventilation systems are recommended to provide an acceptable level of supplied ventilation rates based on the product of designed occupants levels and the ventilation requirement per person. However, during a given day, ventilation systems are still operated based on the designed occupants levels instead of actual levels based on monitoring, often resulting in a waste of energy [7]. In order to provide realistic ventilation flow rates, it is of great importance to know indoor pollutant concentration field quickly and efficiently resulting from any type of indoor-pollutant-source distribution, further facilitating the design and control of indoor ventilation systems for practical application.

For the prediction of the indoor pollutant concentration with stationary source conditions, the low-dimensional linear ventilation models (cf. Cao and Meyers [1,4]) have been developed. In this study, we develop reduced-order models for transient pollutant dispersion, with a focus on the pollutant decay problem. Then, we formulate the solution in terms of a matrix exponential, and show that its rep-
representation can be truncated to only a few dominant eigenmodes. In Sec. 2, a reduced-order ventilation model is derived. In Sec. 3, the methodology is demonstrated on a simple 2D ventilation test case. Conclusions are drawn in Sec. 4.

2 Derivation of a reduced-order pollutant-decay model

In the present work, we focus on the transient ventilation cases, particularly on the elaboration of a representation of the pollutant decay problem. Consider following decay problem of concentration $c$

$$\frac{dc}{dt} + \nabla \cdot (uc) - \nabla \cdot (D \nabla c) = 0, \quad x \in \Omega; \quad t \geq 0$$

$$c(x, 0) = c_0(x).$$

where $c_0$ is the initial concentration, and further $c_0(x, t), \quad c(x, t) \geq 0$.

The spatial discretization of Eq. (2.1), e.g., using a finite-volume approach, leads to a large coupled system of Ordinary Differential Equations (ODEs) that can be cast in following form,

$$\frac{dc}{dt} + A \cdot c = 0,$$

$$c(0) = c_0.$$  

Here $c \in \mathbb{R}^n$ is a long vector containing the discrete concentrations at every cell in the solution domain (with $n$ cells). Further, $A \in \mathbb{R}^{n}$ is a matrix that represents the discretization of the operator $\nabla \cdot u - \nabla \cdot D\nabla$, including the spatial boundary conditions [8]. If appropriate spatial boundary conditions are used in Eq. (2.2), the matrix $A$ is non-singular, i.e. a valid set of boundary conditions leads to a unique solution of the stationary system.

The solution of a linear system of first-order ODEs such as Eq. (2.2) can now be expressed using the matrix exponential $\exp(At)$ To further elaborate this, $A$ is diagonalized. To that end, we presume that the matrix $A$ has $n$ linearly independent eigenvectors $[1, 11]$. Thus, $A = V \Lambda V^{-1}$, with $\Lambda$ a diagonal matrix containing the eigenvalues $\lambda_j$ of $A$, and $V$ a matrix of which the columns are the eigenvectors $v_j$ ($j = 1 \cdots n$) of $A$. Further, the rows of $V^{-1}$ are the eigenvectors $v_j^T$ of $A^T$ i.e. it is easy to verify that $A^T(V^{-1})^T = \Lambda (V^{-1})^T$ and the vectors $v_j$ and $v_j^T$ form a biorthogonal basis, i.e. $v_j^T v_j = \delta_{jj}$ [1]. (Note that for symmetric matrices, $v_j = v_j^T$, but since the convection operator is non-symmetric, $A$ will also be a non-symmetric matrix.) Using these definitions, the solution to Eq. (2.2) is expressed as $[1, 9]$
\[ c(t) = \exp(At) c_0 = V \exp(At) V^{-1} c_0 = \sum_{j=1}^{n} (v_j^T c_0 \exp(\lambda_j t) v_j, \quad (2.3) \]

In the context of three-dimensional dispersion simulations, with domains that contain hundred thousands or millions of cells \((n=10^5-10^6)\), it is not feasible to use Eq. (2.3) directly to solve Eq. (2.2), since the eigenvalue decomposition of \( A \) and \( A' \) would require excessive computational times, proportional to \( n^3 \). However, Eq. (2.3) serves as an interesting starting point to construct a low-dimensional model. To that end, it is important to realize that Eq. (2.3) is a decay problem, so that \( c \to 0 \) for \( t \to \infty \). Thus, the real parts of all eigenvalues of \( A \) are negative, and can be arranged in decreasing order, such that \( 0 > \lambda_{r,1} \geq \lambda_{r,2} \geq \lambda_{r,3} \geq \cdots \).

The construction of a reduced-order pollutant-decay model now proceeds by truncating Eq. (2.3) to the first \( q \) terms, i.e.

\[ c(t) \approx \sum_{j=1}^{q} a_j \exp(\lambda_j t) v_j, \quad (2.4) \]

With \( a_j = (v_j^T c_0) \). This requires \( t \) to be sufficiently large such that \( a_{q+j} \exp(\lambda_{r,q+j} t) \| v_{q+j} \| \approx 0 \) (\( j \geq 1 \)). Provided that \( a_j \), and \( v_j \) are of order unity, a rule of thumb is to take \( t > \tau_q = 5/|\lambda_{r,q+1}| \), leading to \( a_{q+j} \exp(\lambda_{r,q+j} t) \| v_{q+j} \| < 6.7 \times 10^{-3} \). Thus, when it is sufficient from a practical point of view to resolve \( \tau_q \) as fastest time scale in the solution, it may be sufficient to include the first \( q \) eigenvector pairs only in the truncation. In particular if \( q \) is not too big, efficient iterative eigenvalue algorithms can be employed to obtain \( \lambda_j, v_j, \) and \( v_j^* \). For the example application in section 3.2, \( q = 4 \) is sufficient, and we employ the ‘shift and invert’ algorithm [5] to estimate the first 14 eigenvalues, and eigenvector pairs. This algorithm scales linearly with \( n \), and is specifically designed for large sparse systems.

### 3 Results and Discussion

#### 3.1 RANS simulation: details of the set-up

To test the methodology proposed in Section 2, we perform a RANS simulation of a simple two-dimensional ventilation benchmark case, using the open-source CFD software OpenFOAM. A detail of the geometry, and the computational mesh used for the CFD is provided in Fig. 1.

The computational mesh is block hexahedral structured (cf. Fig. 1) containing a total of 34000 cells (i.e. \(160 \times 190 \) in the main block, and \(60 \times 60 \) cells in the outlet). The slot-Reynolds number \( Re_s \) (defined using inlet velocity \( U_0 \), and the
inlet-slot height 0.6 m) corresponds to 4200. At the inlet, a uniform velocity profile is applied with \( U_0 = 0.4 \text{ m/s} \). The turbulence intensity is set at 10%, and a turbulent length scale of 0.02 m is chosen. The non-dimensional ventilation equations are solved in RANS formulation, and closed with a low-Reynolds number \( k - \varepsilon \) model [3,6].

Two RANS simulations are performed. First of all, a stationary simulation is executed that determines the flow solution and the initial concentration profile. To this end, a point source is used located at \((x,y) = (4.5,2.0)\) (cf. Fig. 2). Secondly, a pollutant-decay simulation is executed starting from the initial concentration profile, and using the stationary background flow. We then discuss eigenvalues and eigenmodes of the test case in the next section.

### 3.2 Discussion of largest eigenvalues and eigenvectors

In the current section, we present the dominant eigenmodes associated with the selected test case, and discuss their physical relevance. Based on the velocity and the turbulent diffusion field, obtained from the stationary flow solution, the matrix \( \mathbf{A} \) is now generated (cf. Eq. 2.2). Next, to obtain the eigenvalues and eigenmodes of \( \mathbf{A} \), a parallel C code is written, that reads \( \mathbf{A} \) from disk, and employs the SLEPc library [10] for the eigenvalue analysis. In particular, the ‘shift and invert’ algorithm is used [5], that is specifically designed for the determination of the dominant eigenvalues and eigenvectors of large sparse matrices.

#### Discussion on the largest eigenvalues

Fig. 3 shows the 14 largest eigenvalues of the matrix \( \mathbf{A} \) in the complex plane. Apart from eigenvalues that are real, we also find complex eigenvalues. These come in complex conjugate pairs, and in Fig. 3, we explicitly accounted for that by giving them numbers \( j(a), j(b) \) respectively (e.g., \( j=3 \)). As discussed earlier, only the real part of eigenvalues corresponds to the concentration decay. The larger the real part (closer to zero), the slower the corresponding eigenvector decays. From Fig. 3 it is obvious that the magnitude of eigenvalues' real part is negative. The corresponding eigenvectors are now further discussed.
The first eigenmode

First we focus on the first eigenmode that represents the concentration distribution at infinite time. In Fig. 4 (a) this eigenmode is displayed in color, and normalized by its largest value. In Fig. 4, we also plotted the streamlines of the flow field. It is very clear that this flow field impacts on the shape of the eigenvector. In Fig. 2, we plotted the velocity magnitude, and the total diffusivity. In particular in regions where both velocity and diffusion are small, we find high values for the first eigenmode. In these regions, pollution decays the slowest.

Finally, we emphasize that the first eigenmode as shown in Fig. 4 (a) is positive. This is a requirement since for $c_0 > 0$, and $t \to \infty$, $c_0 > 0$ should hold.

Real eigenmodes

We further focus on eigenmodes containing a real part only, as seen in Fig. 4 (a), (b), (e) and (f), representing the 2nd, 4th and 5th dominant eigenmodes (corresponding to the eigenvalues shown in Fig. 3). Each of them are normalized by the largest absolute value of its corresponding eigenvector. Unlike the first eigenmode, higher modes can have both positive and negative values. However, given $c_0 > 0$, the sum of all eigenmodes needs to be higher than 0 at any time. Thus the higher eigenmodes can be interpreted as corrections to the first eigenmode for $t < \infty$.

Fig. 4 (b) shows noticeable effects only in the upper corner of recirculation region. This is due to the fact that the turbulent mixing also happens along the flow trajectory between the primary recirculation and secondary recirculation region, thus potentially allowing for part of the pollutant to enter the secondary recirculation. This eigenmode further serves as a correction to the first eigenmode.

In Fig. 4 (e) and (f) (corresponding to the 4th and 5th eigenmodes), we observe that the eigenmode is prominent only in a very small corner region as shown by the zooms of Fig. 4 (e) and (f). We conclude that these two eigenmodes play a negligible role in the dispersion problem. We also investigate several higher eigenmodes, and similar behavior occurs.
Fig. 3: The 14 largest eigenvalues of matrix $A$ in the complex plane.

Fig. 4: Streamlines and colour plot of 5 dominant eigenmodes, described by a set of normalized eigenvectors: [(a), (b), (c), (f): the $1^{st}$, $2^{nd}$, $4^{th}$, $5^{th}$ dominant eigenvectors, each normalized by the largest absolute value of its corresponding eigenvector; (c),(d): respectively corresponding to the real part and imaginary part of the 3(a) dominant eigenvector (a complex eigenmode), normalized by the largest value of its eigenvector; the 3(b) eigenmode and the 3(a) eigenmode are a complex conjugate pair, so not shown here]
Thus the overall conclusion is that the first 4 dominant eigenmodes ($q = 4$, cf. Sec. 2) are sufficient to estimate the pollutant concentration decay process. The influence of the complex eigenmode is further discussed below.

**Complex eigenmodes**

After considering the eigenmodes having only a real part, we now look at the eigenmodes having both a real part and imaginary part. The complex eigenmodes $3(a)$ and $3(b)$ (in Fig. 3) represent a complex conjugate pair. They share the same magnitude of the real part and imaginary part but having opposite signs for the imaginary part. Only one of the eigenmodes, i.e., $3(a)$ is considered. The real part and imaginary part of this eigenmode are shown in Fig. 4(c) and (d), normalized by the largest value of its eigenvector.

Fig. 5 represents the periodic cycle corresponding with the complex eigenmodes for $3(a)$ and $3(b)$ for one period and with phase increments of $\pi/2$. We can clearly see that the complex eigenmodes $3(a)$ and $3(b)$ participate in the primary recirculation process in the enclosure.

**4 Conclusions**

Reduced-order ventilations models were derived for pollutant decay problems. To test this approach, a simple 2D ventilation case was considered. Using this case, two RANS simulations were performed. At first we conducted a stationary source simulation that determined the flow solution and the initial concentration profile.
Based on the stationary background flow, we performed a pollutant-decay simulation starting from the initial concentration field. Later we discussed the impacts of the first few dominant eigenmodes (including both real and complex eigenmodes). We found that the first 4 eigenmodes are sufficient to predict the pollutant concentration decay. We also found that the complex eigenmodes play a very important role in primary recirculation processes.

5 References