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Stable reduced-order models for pollutant dispersion in the built environment

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ABSTRACT

In order to limit the impact of accidental releases of hazardous pollutants into the atmosphere, there is a need for an accurate near-range atmospheric dispersion modeling approach that is suitable for on-line risk management. Computational Fluid Dynamics (CFD) has proven to be a promising tool for atmospheric dispersion studies at the near-range. However, the relatively long computing times currently prohibit the use of CFD for real-time purposes. Therefore, we present in this work an effective model reduction method that is based on the projection of the original model, which solves the transient advection-diffusion equation on a steady background velocity field, onto a Krylov subspace by means of the Arnoldi algorithm. This allows to construct a reduced order model (ROM) from an accurate CFD model that is guaranteed to be stable. The algorithm is formulated in such a way that the ROM can be derived using any CFD software package, commercial or non-commercial. The accuracy of the ROM is illustrated by performing a series of simulations of a time-dependent pollutant release at the Doel nuclear power station, located to the north of Antwerp (Belgium). A comparison between the results obtained using the ROM after initialization, and the original CFD model shows a reduction of a factor of 2500 in computational time, leading to a ROM that runs 25 times faster than real-time without a significant loss in accuracy. In terms of computational cost, the ROM is a factor 10^5 less expensive than the original CFD model.

1. Introduction

The impact of accidental atmospheric releases of hazardous pollutants on the health of the people exposed remains of serious concern [1]. Predicting the time-dependent dispersion of such releases in the atmosphere through the use of numerical models can help to develop plans of response to emergencies. Furthermore, when the runtime is sufficiently short, these models can be used in on-line risk management tools (see, e.g., Ref. [2], or Ref. [3]). While Gaussian-based and Lagrangian models are well established for the latter, Leelőssy et al. [4] identified that there is currently no accurate near-range atmospheric dispersion modeling approach available which complies with this short runtime.

Computational Fluid Dynamics (CFD) has proven to be a promising technique for atmospheric dispersion studies at the near-range [5–8]. This is in particularly true for the built environment where the complex geometry can result in complex dispersion patterns [9–12]. Unfortunately, CFD-based models require relatively long computing times which currently prohibit their use for real-time purposes [13,14]. In this context, Senocak et al. [15] focused on reducing the simulation time by improving the numerical methods and parallel computing strategies. Gowardhan et al. [16] chose to trade some of the accuracy for a gain in simulation speed by simplifying the model. In the current work, we take a different approach by developing a reduced order model (ROM) from a CFD model, thereby greatly reducing the computational time. We consider the particular case of a neutral buoyant gas, that is injected with a time-dependent source rate and dispersed given known steady wind conditions and site geometry. In such a system, the background velocity field can be precomputed using CFD, and used as an input to a three-dimensional time-dependent convection-diffusion equation with a transient source term.

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The goal of model order reduction (MOR) is to reduce the degrees of freedom (DOF) of a large size model to a very small size while maintaining the key behavior of the model [17]. Extensive discussions on MOR methods are presented by Baur et al. [17], Lucia et al. [18] and Antoulas et al. [19]. In the following, we focus on MOR methods dedicated for sparse, linear time-invariant systems such as we encounter in our work (cf. section 2.1). The DOF for CFD applications is typically in the order of 10^6 and higher. This is far beyond the practical limit for Truncated Balanced Realization and Hankel Norm Approximation methods, two frequently used ROM methods for linear, time-invariant systems [20]. Instead, Krylov-subspace projection-based ROM methods have shown to be a viable option for such systems [17,20,21]. Many algorithms exist for construction of the Krylov subspaces (see, e.g., Ref. [22] or Ref. [23]) but two frequently encountered algorithms are the Arnoldi method and the Lanczos method. Nour-Omid et al. [24] compared both methods for the solution of convection-diffusion problems in a Finite Element Method framework. They concluded that the Arnoldi is the method of choice for convection dominated problems. Other examples of the application of the Arnoldi method are presented by Woodbury et al. [25] with the simulation of the contaminant transport in an aquifer, Zhang and Woodbury [26] with a study on the contaminant transport in porous media, Willcox et al. [27] with the development of a ROM for turbomachinery and Wang et al. [28] who developed a ROM for the three-dimensional thermal analysis of microfluidic systems. The degrees of freedom in these applications were all limited to $10^3 - 10^5$, which is considerably lower than required for three-dimensional pollution-dispersion studies as considered in the current work. Nevertheless, all these studies demonstrated significant reductions in required computational cost when solving the corresponding ROM.

Therefore, we apply the Arnoldi method to the simulation of pollutant transport in a built environment. We show that the resulting ROM is guaranteed stable and suitable for faster than real-time atmospheric dispersion assessments. In addition, the algorithm for the construction of the ROM is formulated independently from the choice of CFD solver, such that it is applicable to both open-source and commercial CFD software packages. The effectiveness of the reduced-order model is demonstrated based on a simulation of a time-dependent pollutant release at the Doel Nuclear Power Station, comparing the ROM results to the high-resolution CFD.

This paper is further organized as follows. First, in section 2, we present the model order reduction methodology and the pollutant dispersion model. Next, in section 3 we detail the simulation cases considered in the current work and the numerical set up of our simulations. Simulation results are discussed in section 4. Finally, conclusions are presented in section 5.

2. Methodology

In the current section we briefly introduce the continuous and discrete formulation of the pollutant dispersion model in section 2.1. Next, the construction of the ROM is presented in section 2.2.

2.1. Pollutant dispersion model

Consider the three-dimensional dispersion of a non-buoyant, non-reactive gas in a steady, thermally neutral boundary layer, for a constant wind direction, and known site geometry. In this situation, the three-dimensional velocity field $\langle \boldsymbol{u} \rangle(\boldsymbol{x})$ can be obtained from a standard CFD model, e.g., either based on Reynolds-averaged Navier–Stokes simulations or large-eddy simulations (for practical details, cf. section 3.2). The dispersion is then further modeled using a time-dependent three-dimensional advection-diffusion problem. Neglecting the small effect of molecular diffusion, the evolution of the pollutant concentration is described by

$$\frac{\partial c}{\partial t} + \nabla \cdot (\langle \boldsymbol{u} \rangle c) = -\nabla \cdot \langle \boldsymbol{u}' c' \rangle + S \tag{1}$$

where c is the concentration, and S the pollutant source term. We model the turbulent diffusion $\langle \boldsymbol{u}' c' \rangle$ with an eddy-diffusivity approach, i.e.

$$-\langle \boldsymbol{u}' c' \rangle \approx \frac{\nu_t}{Sc_t} \nabla c \tag{2}$$

with Sc_t the turbulent Schmidt number, and ν_t the eddy viscosity. The latter is also straightforwardly obtained from a precomputed flow simulation. In the current study we employ $Sc_t = 0.9$ (see, e.g., Ref. [29] for a discussion on values for the turbulent Schmidt number).

Spatial discretization of Eq. (1), e.g., using a finite-volume approach, results in a large coupled system of ordinary differential equations. This system can be written as

$$\frac{d\tilde{c}}{dt} = A\tilde{c} + bs \tag{3}$$

where $\tilde{c}(t) \in \mathbb{R}^n$ is the solution vector containing the concentration of every cell in the domain, $b \in \mathbb{R}^n$ is the source vector containing the contribution of every cell to the pollutant source and $s(t)$ is the source magnitude input. In addition, the sparse matrix $A \in \mathbb{R}^{n \times n}$ is the discrete representation of the advection and the diffusion operator, including the spatial boundary conditions. When set up properly, this matrix is negative-definite. Note that in practice, this matrix is not explicitly available, but indirectly coded in the CFD software used to solve Eq. (1).

Algorithm 1 One-sided Arnoldi algorithm to construct a basis of $\mathcal{K}_r(A^{-1}, A^{-1}b)$.

1. Initialize:
   (a) Solve for $\tilde{v}_1$[†]: $A\tilde{v}_1 = b$
   (b) Set: $v_1 = \frac{\tilde{v}_1}{\|\tilde{v}_1\|}$
2. For $i = 2 \ldots r$ do:
   (a) Solve for $\tilde{v}_i$[†]: A $\tilde{v}_i = v_{i-1}$
   (b) Orthogonalize $\tilde{v}_i$: for $j = 1 \ldots i-1$
   $h = \tilde{v}_i v_j$
   $\tilde{v}_i = \tilde{v}_i - h v_j$
   (c) Normalize: $v_i = \frac{\tilde{v}_i}{\|\tilde{v}_i\|}$
3. Set $V = [v_1 v_2 \ldots v_r]$
4. Construct $A_r = V^T A V$

[†] This step can be performed using the CFD package by imposing b or v_{i-1} as source vector in Eq. (3) and solving for the steady state solution.