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Abstract—In this paper, we propose a POD-based technique that is suitable for the design of reliable observers for the estimation of velocity field and contaminant flow for Navier-Stokes flow. POD modes are constructed using the method snapshot. Karhunen-Loeve (Galerkin) projection to develop a reduced-order model obtained by projecting the velocity field onto the most important POD modes. The resulting finitedimensional dynamical system is suitable for the design of nonlinear observers. The estimate of the velocity field is then used to estimate the concentration field of a contaminant from the 2D advection-diffusion equation. The prime application considered is the estimation of airflow and contaminant flow in building systems. A 2D simulation example is provided to demonstrate the applicability of the technique.

I. INTRODUCTION

Flow control and optimization research has been very active over the last few years. In contrast, the flow estimation problem has not been considered to such an extent. One of the major challenges of the NS equations is the fact that they are nonlinear. In most cases, a linearized version of the Navier-Stokes equation is considered. Using existing tools from linear infinite dimensional system control ([7],[8]), one can obtain a number interesting results for the control and estimation of flow systems. Kalman filter based approaches have been recently reported in [9] and [10].

The state estimation problem is particularly complex since the number of available sensors are generally quite limited and sensor placement is often restricted due to the lack of accessibility and extreme conditions (not suitable for sensor viability). The knowledge of 2D and 3D NS velocity field has multiple applications in very diverse areas. In building systems, the knowledge of the velocity field in building systems allows one to monitor contaminant flows inside the building and to control air quality. Velocity field estimation play an important role in meteorological applications especially in cases where one is attempting to estimate contaminant flow using basic ground measurements. In general contaminant flow estimation is based on the assumption that the velocity field is known and constant. Under this assumption, the component mass balance becomes linear and hence the estimation can be conducted using purely linear techniques. In many applications, as in building systems, the variations in the velocity field can be significant and thus, the estimation of contaminant based on a steady-state assumption may be

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seriously compromised. POD-based techniques are generally more suitable for nonlinear system. Once a projection into a finite dimensional subspace is obtained (by the method of snapshots for example), the nonlinear NS equations can be projected onto the subspace using Galerkin projection (a.k.a. Karhunen-Loeve projection). The Galerkin projections express the distributed state variables as linear combinations of the POD modes. By setting the variables in this form and substituting to the original equations, a set of nonlinear ordinary differential equations is obtained for the coefficients. The main advantage of the Galerkin projection is that it preserves the nonlinearity of the complex system in the form of a low-dimensional set of nonlinear ordinary differential equations. The application of POD-based technique in simple geometry has been recently demonstrated in Rowley [2]-[5]. In [14], POD-based estimation techniques were developed for the estimation of velocity field in building systems. In this study, we pursue the work presented in [14] and propose the use of POD-based approach for the estimation of velocity field and contaminant flow in building systems. The effectiveness of the technique is demonstrated for a 2D flow problem. It is shown that both convective and diffusive contaminant flow can be accurately estimated along with the velocity field using a finite-dimensional estimator of low dimensions. The paper is structured as follows. In Section II, the POD-based approach is applied to the estimation of velocity field. The estimation of contaminant flow is described in Section III. Section VI presents simulation results of 2D room case study followed by brief conclusions in Section VII.

II. VELOCITY FIELD ESTIMATION

In this section of the paper, we consider the estimation of velocity fields in air flow in building systems. For the purpose of this study, we assume that the airflow velocity field dynamics are governed by the incompressible Navier-Stokes equation given by:

where $u: \Omega \times \mathbb{R} \to \mathbb{R}^3$ represents the velocity field taking values over a spatial domain Ω , p is the pressure field, $\nu = 1/\text{Re}$, Re is the Reynolds number. Here it is assumed that the velocity and pressure fields are defined on a closed-subset of \mathbb{R}^3 and take values on a normed space \mathcal{V} . This equation constitutes a scaled formulation of the Navier-Stokes equation where the velocities are scaled by a factor U, time by U/L, the viscosity by ρUL and the pressure by ρU^2 where ρ is the density, U and L are nominal velocities and length.

The incompressible flow assumption is justifiable for the set of conditions considered for the modeling of airflow in commercial buildings. We note that the approach described below can be directly applied to the compressible flow assumption (as demonstrated in [2]-[5]).

A. POD Based Model Reduction

In POD based model reduction, the velocity field u(x,t) is expressed as an expansion in the POD modes $\phi(x)$ defined on the spatial domain Ω . (Note that depending on the application, temporal models $\psi(t)$ may be more appropriate). The expansion is given as:

$$u(x,t) = \sum_{j=1}^{n} a_j(t)\phi_j(x)$$
 (2)

In general, the decomposition is taken over a Hilbert space H, the space of smooth divergence-free vector-valued functions on Ω . The choice of inner product becomes a crucial aspect of the decomposition. In the incompressible flow approach however, the standard inner product

$$\langle u , v \rangle = \int_{\Omega} u(x) \cdot v(x) dV$$
 (3)

where $u(x) \cdot v(x)$ represents the standard dot product between vectors u(x) and v(x) in Euclidean space, dV is a volume element.

The basis of the technique described here is to restate the Navier-Stokes equation in terms of the modal decomposition (2). Assuming that $div(\phi_i) = 0$ (i = 1, ..., n), substitution of (2) in (1) yields

$$\sum_{i=1}^{n} \dot{a}_i(t)\phi_i(x) = -\left(\sum_{j=1}^{n} a_j(t)\phi_j(x) \cdot \nabla\right) \sum_{k=1}^{n} a_k(t)\phi_k(x)$$
$$+\nu \sum_{i=1}^{n} a_i(t)\nabla^2\phi_i(x) - \nabla p \qquad (4)$$

Projecting onto the space of POD modes leads to,

$$\langle \sum_{k=1}^{n} \dot{a}_{k}(t)\phi_{k}(x),\phi_{i}(x)\rangle = -\langle \left(\sum_{j=1}^{n} a_{j}(t)\phi_{j}(x)\cdot\nabla\right)\sum_{k=1}^{n} a_{k}(t)\phi_{k}(x),\phi_{i}(x)\rangle + \nu\langle \sum_{k=1}^{n} a_{k}(t)\nabla^{2}\phi_{k}(x),\phi_{i}(x)\rangle - \langle \nabla p,\phi_{i}(x)\rangle.$$
(5)

By orthogonality of the modes

$$\langle \phi_i(x), \phi_j(x) \rangle = \begin{cases} 1 & i=j \\ 0 & i\neq j \end{cases}, \tag{6}$$

it follows that (5) reduces to the following set of ordinary differential equations:

$$\dot{a}_{i}(t)\langle\phi_{i}(x),\phi_{k}(x)\rangle = -\sum_{i=1}^{n}\sum_{j=1}^{n}a_{i}(t)a_{j}(t)\langle(\phi_{j}(x)\cdot\nabla)\phi_{i}(x),\phi_{k}(x)\rangle + \nu\sum_{i=1}^{n}a_{i}(t)\langle\nabla^{2}\phi_{i}(x),\phi_{k}(x)\rangle - \langle\nabla p,\phi_{k}(x)\rangle \quad (7)$$

which reduces to

$$\dot{a}_{k}(t) = -\sum_{i=1}^{n} \sum_{j=1}^{n} a_{i}(t)a_{j}(t)\langle (\phi_{j}(x) \cdot \nabla)\phi_{i}(x), \phi_{k}(x)\rangle +\nu \sum_{i=1}^{n} a_{i}(t)\langle \nabla^{2}\phi_{i}(x), \phi_{k}(x)\rangle - \langle \nabla p, \phi_{k}(x)\rangle.$$
(8)

Equation (8) provides the basis for the design of the observer. Given a set of representative POD modes, the reduced-order system of ordinary differential equations constitutes a description of the fluid flow dynamics. Thus by building an observer for system (8), an (indirect) observer of the fluid flow velocity field u(x,t) is obtained.

B. POD modes

The ability to reconstruct the velocity field u(x, t) using estimates of the time-varying coefficients $a_i(t)$ depends completely on the choice of POD modes obtained.

Let \mathcal{H} be a Hilbert space with inner product $\langle \cdot, \cdot \rangle$. It is assumed that a data ensemble is given, $\{u_k \in \mathcal{H} | k = 1, \ldots, m\}$, which provides a representative sample of the system dynamics. In general, the ensemble $\{u_k\}$ is composed of a number of experiments designed to highlight various aspects of the process dynamics. These experiments are typically formed a set of snapshots of the velocity field u_k taken at specific times t_k .

These snapshots are usually obtained using CFD simulation of the process and the times t_k of the snapshots are designed to highlight various aspects of the system dynamics. The snapshots can also be obtained through experiments by placing sensors at predefined locations.

For the purpose of this study, the Hilbert space \mathcal{H} is the set of functions defined on the spatial domain Ω where the fluid flows. (Here the spatial domain is the geometry of a room in a building system). Let S be a subspace of \mathcal{H} of fixed dimension n < m. The projection of any element u_k of \mathcal{H} is given by $P_S u_k$ where P_S is the orthogonal projection operator onto S. The objective of proper orthogonal decomposition is to find a subspace S of fixed dimension n < m such that error $E(||u_k - P_S u_k||)$ is minimized, where $|| \cdot ||$ is the induced norm on \mathcal{H} and $E(\cdot)$ is the expectation operator.

The solution of the optimization problem leads to the eigenvalue problem (see [1] for a detailed development),

$$R\phi = \lambda\phi \tag{9}$$

where $R: \mathcal{H} \to \mathcal{H}$ is the linear operator given by

$$R = E(u_k \otimes u_k^*) \tag{10}$$

where $u^* \in \mathcal{H}^*$ is the adjoint (dual) of a $u \in \mathcal{H}$ and \mathcal{H}^* is the space of functionals $u^*(\cdot) = \langle \cdot, u \rangle$. The operation \otimes represents the standard tensor product. Thus for any u, v and w in $\mathcal{H}, (u \otimes v^*)(w) = u \langle w, v \rangle$.

In practice, the snapshots u_k are a sampled value of the velocity field $u(x, t_k)$ at time t_k evaluated at a finite number, N, of locations x_i (i = 1, ..., N) over the spatial domain Ω . Since, in general, the number of spatial locations N is large, the corresponding spectral decomposition problem can become prohibitively complex.

As an alternative, one can compute the POD modes using the method of snapshots. Starting with an ensemble $\{u_k\}$ (with k = 1, ..., m where $m \ll N$), the POD modes are taken as linear combinations of the elements of the ensemble. That is,

$$\phi(x) = \sum_{k=1}^{m} c_k u_k. \tag{11}$$

Note that this choice is not arbitrary since elements of the range of the linear operator R are by construction in the span of the ensemble $\{u_k\}$.

Rewriting the eigenvalue problem yields

$$Uc = \lambda c \tag{12}$$

where U is a m by m matrix with elements $U_{ij} = \frac{1}{m} \langle u_i, u_j \rangle$. (Thus the problem is reduced to an m dimensional eigenvalue problem. Note that this is true even when the original problem is infinite dimensional.)

In this study, the method of snapshots was used to extract the POD modes from a CFD simulation that yield snapshots over a detailed grid over a small number of time instants.

C. Observer Design

The dynamical system (8 yields a set of quadratic differential equations of the form:

$$\dot{a}_k(t) = L_k a(t) + a(t)^T Q_k a(t)$$
 (13)

where L_k are is a row vector with elements are given by

$$L_{k_i} = \nu \langle \nabla^2 \phi_i(x), \phi_k(x) \rangle \tag{14}$$

and Q_k is an *n* by *n* matrix with elements

$$Q_{k_{ij}} = \langle (\phi_j(x) \cdot \nabla)\phi_i(x), \phi_k(x) \rangle \tag{15}$$

for k = 1, ..., n. In general, the pressure term is ignored. This can be justified as follows. Since the POD modes are such that $div(\phi) = 0$, it follows that

$$\int_{\Omega} \nabla p \cdot \phi_k(x) dV = \int_{\partial \Omega} p \phi_k(x) \cdot \mathbf{n}_{\Omega} dS$$
(16)

where \mathbf{n}_{Ω} represents the unit vector normal to the spatial domain Ω . Hence, the pressure term will vanish altogether over a closed domain ($\phi_k(x) = 0$ on the boundary of Ω , $\partial \Omega$).

It is assumed that several measurements are available. If one assumes that r velocity field measurements are available at r predefined locations, these measurements must first be expressed in terms of the modal decomposition. For example, if one measures the average velocity, $u_{avg}(x_0, t) =$ $(u(x_0, t) + v(x_0, t) + w(x_0, t))$, at a point x_o , then the corresponding measurement becomes

$$u_{avg}(x_0, t) = \sum_{i=1}^{n} a_i(t)(\phi_i^1(x_0) + \phi_i^2(x_0) + \phi_i^3(x_0)) \quad (17)$$

where $\phi_i^j(x)$ represents the j^{th} element of the i^{th} POD mode. Since the POD modes are time independent, the resulting output map can be written in the form

$$u_{avg}(x_0, t) = Ca(t) \tag{18}$$

where C is a 1 by n matrix and a(t) is the n-dimensional vector of time varying coefficients of the Galerkin approximation of u(x,t). In general, the output map will be written as

$$y(t) = Ca(t)$$

which is constructed by expressing the measured quantity using the POD modes.

If pressure is measured at a point x_0 , the pressure can be expressed in modal form as follows:

$$p(x_0, t) = \sum_{i=1}^{n} a_i(t) p_i(x_0)$$
(19)

where $p_i(x_0)$ is the pressure associated to $\phi_i(x_0)$.

Assuming that the available measurements include velocity measurements and pressure measurements, the complete dynamical system considered in this study takes the form:

$$\dot{a}_k(t) = L_k a(t) + a(t)^T Q_k a(t) , \ k = 1, \dots, n$$

 $y(t) = Ca(t)$
(20)

The objective of this study is to consider the design of an observer for the system (20). Assuming that the POD modes provide an accurate description of the features of the flow field, the estimation of the Galerkin coefficients $a_i(t)$ yields an estimate of the velocity field using the expression (2). Note that if the initial conditions $a_i(0)$ are known, then the predictions of the dynamical system (20) will be in agreement with actual value $a_i(t)$ and a good estimate of the flow field should result. However, the initial conditions are generally not known and the value of $a_i(t)$ must be replaced by an estimate $\hat{a}_i(t)$. In addition, the flow system is subject to uncertainties and disturbances that must be filtered in some way.

Given the dynamical system (20) and assuming that the system is observable, one can rely on a number of potential approaches to provide estimates of the Galerkin coefficients. The use of an observer for the estimation of the Galerkin coefficients was proposed in [5] for the design of an feedback control scheme. In order to reduce the complexity of the

observer design, only the linear approximation of (20) was considered. It is clear that a nonlinear observer approach would provide improvement in the performance of the observer. This aspect of the problem is treated in this study.

III. ESTIMATION OF CONTAMINANT FLOW

The observer design for the estimation of velocity fields in building systems can be used for contaminant flow estimation. In the remainder of this paper, we will consider the estimation of concentration fields using the velocity field estimation. Given that div(u) = 0 and assuming the diffusivity of the contaminant is spatially constant, the concentration field dynamics are governed by the advection-diffusion equation given by:

$$\frac{\partial c}{\partial t} = -u \cdot \nabla c + \kappa \nabla^2 c + J_s \tag{21}$$

where $c: \Omega \times \mathbb{R} \to \mathbb{R}$ represents the concentration field, $J_s: \Omega \times \mathbb{R} \to \mathbb{R}$ is the source field and $\kappa = \mathcal{D}/UL$ with \mathcal{D} being the diffusivity coefficient. The velocity and time are again scaled by factors U and U/L, respectively. The concentration and source fields are dimensionless as they are taken as the mass fraction of the contaminant.

IV. POD BASED MODEL REDUCTION

Similar to the velocity field, the concentration field, c(x,t) is expressed as an expansion in the POD modes, $\theta(x)$, defined on Ω . The expansion is given by:

$$c(x,t) = \sum_{i=1}^{p} b_i(t)\theta_i(x)$$
(22)

The decomposition is taken over a Hilbert space \overline{H} , taken to be the space of smooth, real valued functions on Ω with the standard inner product:

$$\langle c_i, c_j \rangle = \int_{\Omega} c_i(x) \cdot c_j(x) dV$$
 (23)

Various inner products involving the gradient and the Laplacian of the concentration fields were tested however the standard inner product produced superior results.

Substitution of (2) and (22) into (21) yields:

$$\sum_{i=1}^{p} \dot{b_i}(t)\theta_i(x) = -\left(\sum_{i=1}^{n} a_i(t)\phi_i(x)\right) \cdot \nabla\left(\sum_{i=1}^{p} b_i(t)\theta_i(x)\right) + \kappa \nabla^2\left(\sum_{i=1}^{p} b_i(t)\theta_i(x)\right) + J_s$$
(24)

Projecting onto the space of POD modes leads to:

$$\begin{split} &\langle \sum_{i=1}^{p} \dot{b}_{i}(t)\theta_{i}(x), \theta_{l}(x) \rangle = \\ &-\langle \sum_{i=1}^{n} \sum_{j=1}^{p} a_{i}(t)b_{j}(t)\nabla\theta_{j}(x) \cdot \phi_{i}(x), \theta_{l}(x) \rangle \\ &+\kappa \langle \nabla^{2} \left(\sum_{i=1}^{p} b_{i}(t)\theta_{i}(x) \right), \theta_{l}(x) \rangle + \langle J_{s}, \theta_{l}(x) \rangle (25) \end{split}$$

By linearity of the inner product and orthonormality of the modes, we have the following set of differential equations:

$$\dot{b}_{l}(t) = -\sum_{i=1}^{n} \sum_{j=1}^{p} a_{i}(t) b_{j}(t) \langle \nabla \theta_{j}(x) \cdot \phi_{i}(x), \theta_{l}(x) \rangle$$
$$+ \kappa \sum_{i=1}^{p} b_{i}(t) \langle \nabla^{2} \theta_{i}(x), \theta_{l}(x) \rangle + \langle J_{s}, \theta_{l}(x) \rangle$$
(26)

The set of differential equations from (26) coupled with the set from (8) can be used to design an indirect observer for both the fluid flow velocity field, u(x,t), and the concentration field, c(x,t).

V. OBSERVER DESIGN

A. Reduced Order Nonlinear System

The overall dynamical system yields the following set of quadratic differential equations:

$$\dot{a}_k(t) = L_k a(t) + a(t)^T Q_k a(t), \quad k = 1, \dots n \dot{b}_l(t) = N_l b(t) + a(t)^T P_l b(t), \quad l = 1, \dots p$$
 (27)

where N_l is a row vector with elements given by:

$$N_{l_i} = \kappa \langle \nabla^2 \theta_i(x), \theta_l(x) \rangle \tag{28}$$

and P_l is an *n* by *p* matrix with elements

$$P_{l_{ij}} = \langle \nabla \theta_j(x) \cdot \phi_i(x), \theta_l(x) \rangle \tag{29}$$

for l = 1, ..., p. The source term is ignored since we assume the source, J_s , is a finite set of point sources or nonzero only on $\partial\Omega$. Hence, we have:

$$\langle J_s, \theta_l(x) \rangle = \int_{\Omega} J_s \cdot \theta_l(x) dV = 0, \quad l = 1, \dots p$$
 (30)

B. Measurements

We assume that the concentration of the contaminants can be measured. Similar to the velocity field measurements, we can relate a concentration measurement at position x_0 and time t to the Galerkin projection coefficients, $b_l(t)$, using:

$$c(x_0, t) = \sum_{i=1}^{p} b_i(t)\theta_i(x_0)$$
(31)

Hence, the vector of all the concentration measurements, $y_{conc}(t)$, can be written as:

$$y_{conc}(t) = \overline{C}b(t) \tag{32}$$

Also, if y_{vel} is the vector of all the velocity measurements, the overall dynamical system is given by:

$$\begin{aligned} \dot{a}_k(t) &= L_k a(t) + a(t)^T Q_k a(t), \quad k = 1, \dots n \\ \dot{b}_l(t) &= N_l b(t) + a(t)^T P_l b(t), \quad l = 1, \dots p \\ y(t) &= \begin{bmatrix} y_{vel}(t) \\ y_{conc}(t) \end{bmatrix} = \begin{bmatrix} C & 0 \\ 0 & \overline{C} \end{bmatrix} \begin{bmatrix} a(t) \\ b(t) \end{bmatrix}$$
(33)

C. Observer Design

The objective of the second half of this study is the design of an observer for (33). In [14], an extended Kalman filter (EKF) was considered for the velocity field estimation. For this system, an unscented Kalman filter (UKF) is applied. Despite being able to better handle nonlinearities using unscented transformations, it was found that an UKF did not significantly outperform an EKF for the dynamical system given in (33).

VI. RESULTS

A. 2D Room Case Study

We consider the application of the observer for (33) in the same two-dimensional room previously studied with a change in the location of the inlet. The inlet was placed on the upper wall and directs contaminated fluid down into the room. Figure 1 depicts the location of the inlet as well as the concentration sensors. The location of the single velocity measurement remains unchanged. As seen in the figure, three concentration sensors were used. The sensors at each of the outlets were used to capture the convective transport of the contaminant, carbon monoxide and the middle sensor captured the diffusive transport towards the middle of the room.



Fig. 1. Geometry of the two-dimensional room.

B. Snapshot Generation and Galerkin Projection

Six separation CFD simulations were used for the generation of the snapshots. The first four started with a zero initial velocity and concentration fields within the room. The inlet velocity and mass fraction of carbon monoxide, were 0.179 m/s and 0.02, 0.179 m/s and 0.07, 0.626 m/s and 0.07 and 0.626 m/s and 0.07. The last two simulations started with the steady state velocity fields from an inlet velocity of 0.223 m/s and 0.626 m/s with zero inlet mass fraction. The snapshots were generated with the inlet mass fraction increased from 0 to 0.015. Two velocity and three concentration POD modes were retained from the snapshots.

The Galerkin projection produced a five-dimensional continuous-time dynamical system which was discretized using a sample time of 5 seconds.

A CFD simulation was used to study the performance of the proposed observer. The simulation started with zero initial velocity and concentration fields and inlet velocity and mass fraction of 0.360 m/s and 0.04, respectively. The initial values of the estimates of the Galerkin projection coefficients were $\hat{a}_1 = \hat{a}_2 = \hat{b}_1 = \hat{b}_2 = \hat{b}_3 = 0$.

C. Velocity Estimation

Figure 2 compares the estimated velocity field to the field from the CFD simulation. The result reiterates the effectiveness of the observer at estimating velocity fields as demonstrated in [14].



Fig. 2. Simulation results for the 2D room case study. Shown are the mean squared velocity fields for the CFD and the estimated velocity field at t = 110 sec. The CFD velocity field is on the left and the estimated velocity field is on the right.

D. Convective Transport Estimation

Figure 3 compares the concentration field from the CFD simulation to the estimated field while convection is the dominate method of transport of the contaminant. The results exhibit the efficacy of the observer at estimating the convective transport of the contaminate throughout the room.



Fig. 3. Simulation results for the 2D room case study. Shown are concentration fields for the CFD and the estimated concentration field at t = 110 sec. The CFD concentration field is on the left and the estimated concentration field is on the right.

E. Diffusive Transport Estimation

Figure 4 compares the CFD and estimated concentration fields when the contaminant has diffused into the middle of the room. The results show that the observer is able to estimate both the convective and the diffusive transport of the contaminant. This is in spite of reducing the Navier Stokes and the advection diffusion equation to a five-dimensional dynamical system. Figure 5 shows the total mean squared error in the estimate of the concentration.



Fig. 4. Simulation results for the 2D room case study. Shown are concentration fields for the CFD and the estimated concentration field at t = 340 sec. The CFD concentration field is on the left and the estimated concentration field is on the right.

VII. CONCLUSIONS

A POD-based observer design method is developed for the estimation of velocity field from the 2D and 3D Navier-Stokes flow and contaminant flow from the 2D advectiondiffusion equation. In building systems, the POD-based ap-



Fig. 5. Total mean squared error in the estimate of the concentration field for the 2D room example.

proach provides very simple low-order representation of the flow that are both accurate and reliable.

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