EFFECT OF FINITE-DIMENSIONAL APPROXIMATIONS ON OBSERVABILITY ANALYSIS OF DISTRIBUTED PARAMETER MODELS

Abhay Singh and Juergen Hahn

Artie McFerrin Department of Chemical Engineering
Texas A &M University, College Station, TX 77843-3122

Abstract: This paper investigates the effect of different discretization schemes for observability analysis of distributed parameter models. While it is common knowledge that approximating an infinite-dimensional model can introduce non-physical numerical diffusion or numerical oscillation in the dynamics of finite dimensional approximation of the distributed parameter system, less attention has been paid to the effect that these approximations have on conclusions drawn about observability and controllability of the system. This paper addresses this point and presents a detailed analysis of results obtained for three approximation schemes for first-order hyperbolic partial differential equations (PDEs). The different, and sometimes misleading, conclusions that can be drawn for the three approximation schemes are discussed in detail and the analysis is illustrated with a numerical example. The case study illustrates the point that a model which may approximate the dynamic behavior of the distributed system accurately may not necessarily correctly reflect observability of the original distributed system.

Keywords: Observability, Distributed parameter systems, Discretization.

1. INTRODUCTION

Observability analysis is one of the key steps for designing observers or for computing measurement structures for state estimation. While the tools for observability analysis of linear and nonlinear lumped parameter models are well developed, the same is not true for processes described by PDEs. There are no available techniques for observability analysis of nonlinear infinite-dimensional systems and even the tools developed for linear distributed parameter models are rarely used due to their non-trivial implementation/interpretation (Delatre, et al., 2004). As observability for distributed parameter system is difficult to compute, the infinite-dimensional model is often approximated by employing finite difference techniques or by the use of orthogonal collocation and observability analysis is performed on the finite-dimensional approximation (Dochain, et al., 1997; Van den Berg, et al., 2000; Waldraff, et al., 1998). While there is a large body of literature on the effect of different approximation schemes for infinite-dimensional models on the accuracy of the model prediction (Finlayson, 1980; Ramirez, 1997), there are almost no publications which investigate the effect of different approximations on observability of a system. Exceptions to this are the works by Waldraff, et al. (1998), and Winkin, et al. (2000), where it has been shown for specific cases and approximations that infinite-dimensional model observability can be inferred from finite-dimensional models. However, there is no work in the literature that directly compares the effect of different discretization schemes on observability analysis of a system. This work addresses this point and presents a detailed analysis of observability results for three different approximation schemes for hyperbolic PDEs. Additionally, a case study comparing different discretization schemes for observability analysis of a distributed parameter model is presented. A backward difference, a central difference scheme and an approximation based on orthogonal collocation are investigated. The results from observability analysis for the different approximations are compared with the ones for the infinite-dimensional approach to illustrate that different, and sometimes misleading, conclusions can be drawn from observability analysis for distributed parameter models depending upon the finite-dimensional approximation that is used.

2. PRELIMINARIES

2.1 Observability analysis of first order hyperbolic partial differential equation models.

Observability of first order hyperbolic PDEs can be determined by tools derived from characteristic theory (Goodson and Klein, 1970; Yu and Seinfeld, 1971). In case of a first-order hyperbolic flow process given by:

$$\frac{\partial x(z,t)}{\partial t} = \alpha \frac{\partial x(z,t)}{\partial z} + \beta x(z,t) \qquad x(0,t) = x_0 \qquad 0 \le z \le 1 \tag{1}$$

the solution takes the form

$$\left.\frac{dx}{dt}\right|_0 = \beta x(z,t) \tag{2}$$

along the characteristic lines:

$$t = t_0 - \frac{z}{\alpha} \tag{3}$$

where, $t_0 \ge 0$, $x \in R^n$, $z \in R$, α and β are parameters. If the output of the system (1) is given by:

$$y_i(t) = C_i x(z_i,t), \qquad i = 1,2,\ldots,\gamma \tag{4}$$

then the system defined by (1) and (4) is observable, if each characteristic line defined by (3) intersects a sensor (z_i) and the observability matrix defined by (5) has rank *n*.

$$O = \left[\Phi(t_1,0)^T C_1^T \vdots \ \ldots \ \vdots \Phi(t_\gamma,0)^T C_\gamma^T\right] \tag{5}$$

$\Phi(t,0)$ from equation (5) is the state transition matrix for the system defined in (2) and t_i is computed from equation (3) as:

$$t_i = t_0 - \frac{z_i}{\alpha}, \qquad i = 1,2,\ldots,\gamma \tag{6}$$

for a sensor located at z_i.

2.2 Observability analysis of approximations of infinite-dimensional models.

The infinite-dimensional approach for observability analysis of distributed parameter models is usually difficult to apply in practice (Waldraff et al., 1998). Resulting from this, the model is often approximated by finite difference or orthogonal collocation, followed by observability analysis of the finite-dimensional approximation.

The original distributed parameter model given by (1) can be approximated by a lumped parameter model:

$$\frac{dx(z,t)}{dt} = Ax(z,t) + Bu \tag{7}$$

where, $u \in R^m$, and

$$x = \left[x(z_1,t) \ \ x(z_2,t) \ \ x(z_3,t) \ \ \cdots \ \ x(z_n,t)\right]^T \tag{8}$$

where *n* is the number of spatial discretization points.

Observability analysis is then carried out on the approximate lumped parameter model. If the output of the system defined by (7) is given by:

$$y = Cx \tag{9}$$

where, $y \in R^p$, then the observability matrix (Brockett, 1970):

$$O = \begin{pmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{pmatrix} \tag{10}$$

can be computed in order to determine the observability of the lumped model defined by (7) and (9). If the observability matrix has full rank then the system given by equation (7) and (9) is said to be observable.

However, different discretization schemes can be used to compute the lumped parameter model defined by (7) and (9). If a backward difference scheme is used for discretization of the spatial derivatives, then the first order spatial derivatives for each grid point are expressed as:

$$\left.\frac{\partial x(z,t)}{\partial z}\right|_i = \frac{x(z_i,t) - x(z_{i-1},t)}{\Delta z} \tag{11}$$

where i represents the i th discretization point.
In case of central differences, the first order spatial derivative for each grid point is given by:

$$\left.\frac{\partial x(z,t)}{\partial z}\right|_i = \frac{(x(z_{i+1},t) - x(z_{i-1},t))}{2\Delta z} \tag{12}$$

The finite differences approach of transforming partial differential equations to lumped parameter models is simple to formulate. However, for an accurate description of the system, the infinite-dimensional system may have to be expressed as a system consisting of a large number of ordinary differential equations. One alternative for computing a lumped model is to use functional approximation techniques like orthogonal collocation (Finlayson, 1980; Ramirez, 1997). In this technique, the state variables are expressed as the expansion of an orthogonal polynomial function. The states are defined as:

$$x(z) = \sum_{i=1}^{n+1} a_i P_{i-1}(z) \tag{13}$$

where, n is the number of discretization (or collocation) points. The polynomial $P_n(z)$ is an orthogonal polynomial, e.g. a shifted Legendre polynomial. The collocation points are computed as the roots of the polynomial $P_n(z_j) = 0$. The state expression in (13) can be further written in terms of the collocation point as:

$$x(z) = \sum_{i=1}^{n+1} b_i z^{i-1} \qquad (14)$$

Therefore, the state variable at each collocation point z_j is defined as:

$$x(z_j) = \sum_{i=1}^{n+1} b_i z_j^{i-1} \qquad (15)$$

Accordingly, the derivates are computed at each collocation point by differentiating the above equation with respect to z. In case of a first order derivate, the approximation is given by:

$$\frac{dx}{dz}(z_j) = \sum_{i=1}^{n+1} b_i (i-1) z_j^{i-2} \qquad (16)$$

Similarly, higher order derivative approximations can be computed. The expression for state variable $x(z)$ and its spatial derivative can be written in matrix form as:

$$x(z) = Qb \qquad \frac{\partial x(z,t)}{\partial z} = Tb \qquad (17)$$

where, the matrixces Q and T are given by:

$$Q_{ji} = z_j^{i-1} \qquad T_{ji} = (i-1) z_j^{i-2} \qquad (18)$$

The spatial derivatives can then be expressed as:

$$\frac{\partial x(z,t)}{\partial z} = TQ^{-1} x(z,t) \qquad (19)$$

3. EFFECT OF DISCRETIZATION ON OBSERVABILITY ANALYSIS OF DISTRIBUTED PARAMETER MODELS

As distributed parameter models are usually approximated by finite difference schemes or orthogonal collocation techniques (Ramirez, 1997), it is the purpose of this work to systematically analyze the effect that different discretizations schemes have on the conclusions drawn from observability analysis. As discretization schemes can introduce non-physical numerical diffusion and numerical oscillations in the system dynamics (Wu et al., 1990), incorrect conclusions may be drawn not only for the quality of the approximation but also for observability analysis of distributed parameter models. In fact, it will be shown that for some cases the approximations which result in the best approximation with regard to the time-profile may result in inaccurate information about observability of the system. As this type of analysis can be quite general, a system described by a hyperbolic partial differential equation, as in equation (1), is investigated. Examples of processes modeled by this class of PDEs include heat exchangers, plug flow reactors, and pressure swing adsorption processes (Christofides, 2000).

In order to carry out observability analysis, the system given by equation (1) is approximated by a lumped model described in equation (4). However, the structure of the A matrix in equation (4) depends on the type of discretization employed. If a backward difference scheme is used for discretization of the spatial derivatives, the equivalent lumped parameter model for the system (1) is obtained by writing the following ordinary differential equation for each discretization point:

$$\frac{dx(z_i,t)}{dt} = \alpha \frac{(x(z_i,t) - x(z_{i-1},t))}{\Delta z} + \beta x(z_i,t) \qquad (20)$$

The system of ordinary differential equations (20) for each discretization point can be further simplified and written in states space form as in equation (7), resulting in an A matrix given by:

$$A = \begin{bmatrix} a_{1,1} & 0 & 0 & 0 & \cdots & 0 \\ a_{2,1} & a_{2,2} & 0 & 0 & \ddots & \vdots \\ 0 & a_{3,2} & a_{3,3} & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & 0 & 0 \\ \vdots & \ddots & 0 & a_{n-2,n-1} & a_{n-1,n-1} & 0 \\ 0 & \cdots & 0 & 0 & a_{n-1,n} & a_{n,n} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\alpha}{\Delta z}+\beta & 0 & 0 & 0 & \cdots & 0 \\ -\frac{\alpha}{\Delta z} & \frac{\alpha}{\Delta z}+\beta & 0 & 0 & \ddots & \vdots \\ 0 & -\frac{\alpha}{\Delta z} & \frac{\alpha}{\Delta z}+\beta & 0 & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & 0 & -\frac{\alpha}{\Delta z} & \frac{\alpha}{\Delta z}+\beta & 0 \\ 0 & \cdots & 0 & 0 & -\frac{\alpha}{\Delta z} & \frac{\alpha}{\Delta z}+\beta \end{bmatrix} \qquad (21)$$

where $a_{x,x}$ are scalar, non-zero entries of the A matrix. In order to carry out observability analysis for the lumped parameter model as in equation (7) with the A matrix given by (21), an observability matrix can be computed. If a measurement is placed at the first spatial discretization point, the output matrix in equation (9) is given by

$$C = [1 \quad 0 \quad \cdots \quad 0] \qquad (22)$$

and the observability matrix is computed to be:

$$O = \begin{bmatrix} C \\ CA \\ CA^2 \\ CA^3 \\ \vdots \\ CA^{n-1} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ \frac{\alpha}{\Delta z}+\beta & 0 & \ddots & 0 \\ \left(\frac{\alpha}{\Delta z}+\beta\right)^2 & \vdots & \ddots & \vdots \\ \left(\frac{\alpha}{\Delta z}+\beta\right)^3 & \vdots & \ddots & \vdots \\ \vdots & 0 & \ddots & 0 \\ \left(\frac{\alpha}{\Delta z}+\beta\right)^{n-1} & 0 & \cdots & 0 \end{bmatrix} \qquad (23)$$

The observability matrix has a rank of one for the chosen measurement location. Similarly, it can be shown that the rank of the observability matrix increases as the measurement is moved from the first spatial discretization point to the last discretization point. The rank of observability matrix is two for a measurement at the second discretization point, and three for a measurement at the third discretization point. In case of a measurement at the last discretization point, the output matrix in equation (9) is given by:

$$C = [0 \quad 0 \quad \cdots \quad 1] \qquad (24)$$

and the structure of the observability matrix is given by the following triangular matrix:

$$O=\begin{bmatrix} 0 & \cdots & \cdots & 0 & 0 & 1 \\ 0 & \iddots & \iddots & 0 & -\frac{\alpha}{\Delta z} & \frac{\alpha}{\Delta z}+\beta \\ \vdots & \iddots & 0 & \left(-\frac{\alpha}{\Delta z}\right)^2 & \cdots & \left(\frac{\alpha}{\Delta z}+\beta\right)^2 \\ 0 & 0 & \iddots & \iddots & \iddots & \vdots \\ 0 & \left(-\frac{\alpha}{\Delta z}\right)^{n-2} & \iddots & \iddots & \iddots & \vdots \\ \left(-\frac{\alpha}{\Delta z}\right)^{n-1} & \cdots & \cdots & \cdots & \cdots & \left(\frac{\alpha}{\Delta z}+\beta\right)^{n-1} \end{bmatrix} \quad (25)$$

The determinant of the observability matrix (25) is given by $\left(-1\right)^{\frac{n(n-1)}{2}}(-\frac{\alpha}{\Delta z})^{\frac{n(n-1)}{2}}$. Hence, the observability matrix will have full rank for non-zero α. Therefore, if a backward difference is used for spatial discretization then the system can be observable only if the measurement is placed at the last discretization point.

If a central difference scheme is used for discretization of spatial derivatives, the ordinary differential equation for each discretization point is given by:

$$\frac{dx(z_i,t)}{dt} = \alpha\frac{(x(z_{i+1},t) - x(z_{i-1},t))}{2\Delta z} + \beta x(z_i,t) \quad (26)$$

The structure of the A matrix for the central difference discretization scheme is given by:

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & 0 & 0 & \cdots & 0 \\ a_{2,1} & a_{2,2} & a_{2,3} & 0 & \ddots & \vdots \\ 0 & a_{3,2} & a_{3,3} & a_{3,4} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 0 & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ 0 & \cdots & 0 & 0 & a_{n,n-1} & a_{n,n} \end{bmatrix}$$

$$= \begin{bmatrix} \beta & \frac{\alpha}{2\Delta z} & 0 & 0 & \cdots & 0 \\ -\frac{\alpha}{2\Delta z} & \beta & \frac{\alpha}{2\Delta z} & 0 & \ddots & \vdots \\ 0 & -\frac{\alpha}{2\Delta z} & \beta & \frac{\alpha}{2\Delta z} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 0 & -\frac{\alpha}{2\Delta z} & \beta & \frac{\alpha}{2\Delta z} \\ 0 & \cdots & 0 & 0 & -\frac{\alpha}{\Delta z} & \frac{\alpha}{\Delta z}+\beta \end{bmatrix} \quad (27)$$

In this case the A matrix has a tri-diagonal structure. It should be noted that the entries $a_{x,x}$ in the A matrix (27) will usually be different from the entries in (21). It can be shown that the system defined by (7) with the A matrix from (27) is observable for any measurement location. For example, if the measurement is placed at the first discretization point, then the observability matrix is given by:

$$O=\begin{bmatrix} 1 & 0 & 0 & \cdots & \cdots & 0 \\ \beta & \frac{\alpha}{2\Delta z} & 0 & \ddots & \ddots & \vdots \\ O_{3,1} & O_{3,2} & \left(\frac{\alpha}{2\Delta z}\right)^2 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \left(\frac{\alpha}{2\Delta z}\right)^{n-2} & 0 \\ O_{n,1} & \cdots & \cdots & \cdots & O_{n-1,n} & \left(\frac{\alpha}{2\Delta z}\right)^{n-1} \end{bmatrix} \quad (28)$$

where the entries $O_{X,X}$ in the above matrix represent the non-zero, scalar entries of the observability matrix. The above observability matrix is of lower triangular form and, therefore, the determinant of the above matrix is given by the product of diagonal elements. As a result, the observability matrix will always have full rank for non-zero α. Hence, unlike for the backward difference scheme, the observability matrix can have full rank even if the measurement is placed at the first discretization point. In fact, for central differences, it can be shown that the determinant of observability matrix is given by $\theta\left(\frac{\alpha}{2\Delta z}\right)^{\frac{n(n-1)}{2}}$, where θ is a non-zero scalar number that depends on the sensor location. Hence, the system is always observable for non-zero α, irrespective of the measurement location, if a central difference scheme is used to approximate the PDE.

An alternative for computing a lumped parameter model are functional approximation techniques like orthogonal collocation (Finlayson, 1980; Ramirez, 1997). The state variables are expressed as the expansion of an orthogonal polynomial function using this methodology. The lumped parameter model is obtained by writing the following differential equation for every collocation point or discretization point:

$$\frac{dx(z_j,t)}{dt} = \alpha\left(\sum_{i=1}^{n+1}[TQ^{-1}]_{ji}x(z,t)\right) + \beta x(z_j,t) \quad (29)$$

If the system is written in the states space form shown in equation (7), then the structure of the A matrix is given by:

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \ddots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ a_{n-1,1} & a_{n-1,2} & \ddots & a_{n-1,n} \\ a_{n,1} & a_{n,2} & \cdots & a_{n,n} \end{bmatrix} \quad (30)$$

It should be noted that, although, the symbol $a_{x,x}$ is used in equation (30) that the matrix elements entries are likely different from the ones in equation (21) or equation (27). The A matrix in (30), unlike the A matrix in (21) and (27), can have all non-zero entries. Accordingly, the observability matrix may be of full rank for any measurement location.

From the above illustration of observability analysis of an infinite-dimensional system, it can be inferred that different observability conclusions can be drawn for the same infinite-dimensional system. In the case of a backward difference scheme, hyperbolic partial differential equation models are only observable if the "most downstream" state of the system is measured. However, for a central difference scheme and for models derived using orthogonal collocation, the infinite-dimensional model can be observable for a measurement placed at any discretization point. If an infinite-dimensional approach as presented in Section 2.1 is used, it can be shown that the system can be observable only if measurement is placed at the last discretization point. Therefore, only the backward difference scheme can make accurate predictions about observability of this type of system.

The reason for the different observability results determined for the individual approximation schemes is that the central difference and orthogonal collocation introduce non-physical numerical diffusion in the dynamics of the system and as a result the structure of the *A* matrix changes. Therefore, the system is observable for measurements placed at any location in the system. The backward difference technique for the presented model does not suffer from this drawback and the results are in line with the infinite-dimensional approach, i.e., the system is only observable if the "most downstream" state of the systems is measured. When selecting a discretization scheme it should be kept in mind that the discretization scheme should correctly describe the physics of the process such that the observability analysis is not influenced by phenomena like non-physical numerical diffusion or numerical oscillations.

While the discussion in this paper is focused on observability, it is possible to draw similar conclusions about controllability as the two concepts are closely related.

4. ILLUSTRATIVE EXAMPLE

A model of an isothermal plug flow reactor with first order kinetics is investigated to illustrate the argument presented above. The reactor model is given by:

$$\frac{\partial C_A(z,t)}{\partial t} = -0.04\frac{\partial C_A(z,t)}{\partial z} - kC_A$$
$$C_A(0,t) = 1$$
$$C_A(z,0) = 1 \tag{31}$$
$$0 \le z \le 0.2\,, \quad k = 1$$

The steady state profile of the reactor for different discretization schemes is shown in Figure 1. The number of spatial discretization points of these schemes is the same and was fixed at 10. The central difference approximation and orthogonal collocation provide accurate model predictions for the convective reactor model, which is a result commonly reported in the literature (Ramirez, 1997).

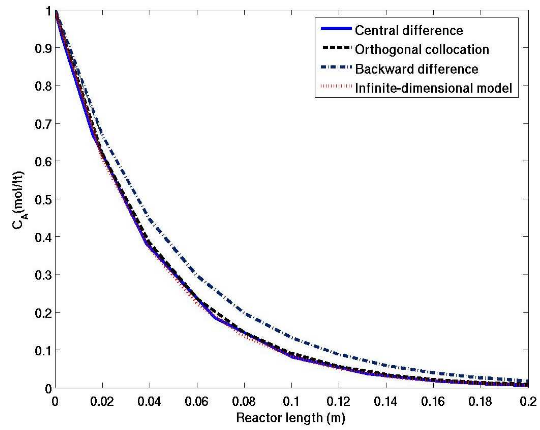

Fig. 1. Comparison of steady state profile of the reactor for different discretization schemes with the infinite-dimensional model.

In comparison, the approximation derived by the backward difference scheme is not as good for this case and requires a larger number of discretization points for model predictions with the same accuracy.

Observability analysis has also been carried out for the infinite-dimensional model and for the different discretization schemes. According to the infinite-dimensional approach presented in Section 2.1, the reactor model will be observable only if the product composition from the reactor is measured, i.e., a sensor is placed to measure the concentration at 0.2m. In the case of the reactor model being approximated by discretizing with central differences or orthogonal collocation, inaccurate observability results are obtained. The observability results for different discretization schemes are summarized in Table 1.

If backward differences are used for the discretization, then the system is only observable for a concentration measurement at the outlet of the reactor. However, in case of central differences or orthogonal collocation, the reactor would seem to be observable for any measurement location. For the central difference schemes, the smallest singular value of the observability matrix remains the same order of magnitude for any location in the reactor, while for orthogonal collocation the smallest singular value increases as the measurement is moved towards the outlet of the reactor. It can be seen from the presented results that central difference and orthogonal collocation introduce non-physical numerical diffusion in a pure convection plug flow reactor model. As a result the lumped parameter model is observable for any measurement in the system, even though this is not the case for the distributed system that it approximates. For this reactor model, a backward difference scheme produces results inline with those obtained from analysis of the infinite-dimensional model.

While the central difference scheme and orthogonal collocation provide an accurate model approximation, these techniques result in increased coupling of the discretized system. The increased coupling, as evident from the structure of the *A* matrix in Section 3, results in non-physical numerical diffusion. As a result, these techniques provide misleading information regarding the observability of the distributed parameter model despite resulting in better accuracy for the description of the concentration profile.

5. CONCLUSION

This work presents an analysis of the effect that the use of different discretization schemes has on observability analysis of infinite-dimensional systems. It is shown that the choice of discretization scheme can not only influence the accuracy of the model prediction, which has been known for a long time, but will also have a direct impact on the conclusions drawn from observability analysis. For a system described by a first order hyperbolic PDE, discretization by backward difference will result in more accurate information about observability than discretization by central difference or orthogonal collocation.

While controllability analysis was not specifically investigated in this work, its conclusions will be affected in a similar manner as the ones drawn for observability analysis.

Table1. Smallest singular value of observability matrix for different discretization schemes

Measurement location (in terms of discretization point)	Smallest singular value of observability matrix		
	Backward difference	Central difference	Orthogonal collocation
1	0	8.99E-04	4.12E-08
2	0	3.71E-04	4.86E-08
3	0	5.74E-04	4.42E-08
4	0	6.45E-04	1.03E-07
5	0	6.28E-04	3.68E-06
6	0	7.11E-04	2.05E-04
7	0	8.79E-04	0.02700
8	0	9.77E-04	0.04990
9	0	9.62E-04	0.04998
10	0.0036	8.89E-04	0.04992

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