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Benaissa Dekhici, Boumediene Benyahia, Cherki Brahim. Model order reduction using Dynamic Mode Decomposition: Application to the Anaerobic Digestion Model N.1 (ADM1): Application to the Anaerobic Digestion Model N.1 (ADM1). CARI 2020 - 15th African Conference on Research in Computer Science and Applied Mathematics, Oct 2020, Thiès, Senegal. hal-02928872

HAL Id: hal-02928872
https://hal.science/hal-02928872

Submitted on 2 Sep 2020

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Model order reduction using Dynamic Mode Decomposition

Application to the Anaerobic Digestion Model N.1 (ADM1)

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ABSTRACT. The Anaerobic Digestion Model No.1 (ADM1) is by far the most detailed model for the simulation and monitoring of Anaerobic Digestion (AD) processes. However, the ADM1 model is not dedicated for control purposes, due to its high dimension with 35 state variables. Dynamic Mode Decomposition (DMD) technique was applied to reduce the ADM1 order, using data generated from the Benchmark Simulation Model No. 2 (BSM2). The method allows to obtain a global linear model with only 7 state variables, which are coherent with dominant dynamics of the ADM1. We show in simulation that we can reconstruct original state variables of ADM1 model.

RÉSUMÉ. Le modèle ADM1 (Anaerobic Digestion Model No.1) est le modèle phénoménologique le plus détaillé de la digestion anaérobie. Néanmoins, ce modèle n'est pas dédié pour le contrôle du processus, à cause de sa complexité. Dans cet article, la technique DMD (Dynamic Mode Decomposition) pour la réduction de modèles a été appliquée au ADM1, en utilisant des données générées par le simulateur Benchmark Simulation Model No. 2 (BSM2). La méthode permet d'obtenir un modèle linéaire global avec seulement 7 variables d'état, qui sont cohérentes avec les dynamiques dominantes de l'ADM1. Nous montrons dans la simulation que nous pouvons reconstruire les variables d'état originales du modèle ADM1.

KEYWORDS : Anaerobic digestion ; ADM1 ; DMD ; Model reduction ; Modeling.

MOTS-CLÉS : Digestion Anaérobie ; ADM1 ; Réduction de modèle ; DMD ; Modélisation

1. Introduction

Anaerobic Digestion (AD) is a promising process for wastewater and waste solid treatment, and biogas production. AD is a very complex process, which involves many bacteria consortia and several biochemical reactions. The Anaerobic Digestion Model N.1 (ADM1) is the most complete phenomenological model of AD. It integrates 35 state variables and more than 130 parameters [1]. Unfortunately, this model is not dedicated for control purposes. In the literature, different technique have been used for the reduction of ADM1 model. Homotopy method based on the eigenvalues association of ADM1 model was applied by Hassam et al. [2] and, a reduced linear model of 14 state variables was obtained. Khedim et al. [3], used a state variables association technics to establish algebraic combinations between variables of a reduced Microalgae Anaerobic Digestion model (MAD) and those of the ADM1 model. A Principal Component Analysis (PCA) technics was used by Garcia-Dieguez et al. [4], on synthetic data from the ADM1 in order to derive a smallest model based only on two biochemical reactions. In this paper, we propose to reduce the ADM1 model, by using Dynamic Mode Decomposition (DMD) technics in order to derive a simple global linear model. First, the ADM1 is presented and the principle of its modeling is discussed. Then, the DMD method is introduced and applied to reduce the ADM1 dimension. Simulation results are obtained and discussed, before conclusion and perspectives are drawn.

2. Anaerobic digestion model No.1

The ADM1 model developed by International Water Association (IWA) Task Group [1], describes in details the AD process. It can be used as a virtual AD bioreactor, for generating data to validate some AD simple models, elaborate optimal control laws or estimate inaccessible state variables. ADM1 describes AD in five steps: disintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis [1]. It considers both biochemical and physicochemical processes (Figure 1), where Organic load is measured in COD unit (Chemical Oxygen Demand), which represents the amount of oxygen needed to decompose organic matters in wastewater.

The ADM1 implementation of a Continuous Stirred Tank Reactor (CSTR) for both liquid and gas phases is described in Figure 2, where the following notations are used for: q = flow, V = volume, ξ = concentration of substrates and biomasses (soluble and particulate components), $\rho_{gas,T}$ = liquid/gas transfer kinetic rates, $S_{gas,i}$ = concentration of gas i, $P_{gas,i}$ = pressure of gas i.

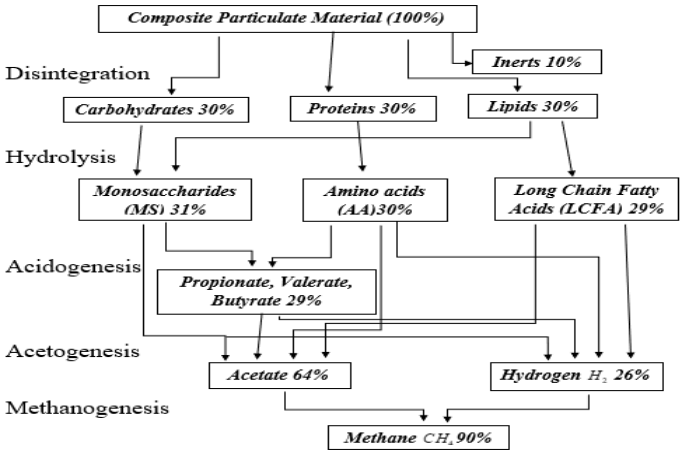


Figure 1 – Reaction paths and COD flux as described in ADM1. [1]

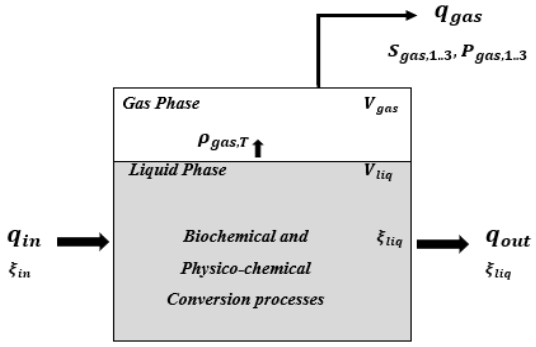


Figure 2 – Schematic diagram of a typical anaerobic CSTR. [1]

The simulation of the ADM1 needs resolution of deferential and algebraic equations (DAE), which are based on the following mass balance law [1].

$$\frac{d\xi_{liq,i}}{dt} = \frac{q}{V}(\xi_{in,i} - \xi_{liq,i}) + \sum_{j=1}^{Nb} \rho_i v_{ij} \tag{1}$$

Where $\xi_{liq,i}$ are the concentrations of components ξ_i in the reactional bulk with input concentrations $\xi_{in,i}$, ρ_i are stoichiometric coefficients for degradation or production of ξ_i, v_{ij} are biological kinetics related to the reaction of ξ_i, Nb is the number of reactions and $D = \frac{q}{V}$ is the dilution rate which represents the control variable. In general, The ADM1 model integrates 19 biochemical kinetic processes, 35 state variables, more than 130 parameters and, simulates substrates degradation processes, specific growth and decay processes of biomasses [5]. It is taken as the state-of-the-art model because of the huge validation success confirmed by the practitioners [6]. A very important application of ADM1 is its implementation in the Benchmark Simulation Model N.2 (BSM2), in order to test control strategies and supervise virtual processes [7]. In this paper, we used the BSM2 to generate virtual data, which will be used by DMD method to derive a simple global linear model from the ADM1.

3. DMD Algorithm

Dynamic Mode Decomposition (DMD) is a new data-driven technique, used to obtain global linear models with reduced order from higher dimensional systems as the ADM1. The DMD principle is collecting snapshots of data x_k from a dynamical system at sample time $t_k, (k = 1, 2, 3...m)$ and then, generating a reduced model which represents the most coherent and dominant dynamics of the original system. The DMD algorithm can be considered as a regression of linear dynamics represented by the scheme below (2) and, it is the result of a combination between spatial dimensionality reduction and Fourier transform in time [8].

$$x_k \xrightarrow{A} x_{k+1} \tag{2}$$

The operator A is a linear combination between x_k and x_{k+1}, which is chosen so that the least square criterion $\|x_{k+1} - Ax_k\|_2$ is minimized for $k = 1, 2, 3...m - 1$. The DMD method can be easily applied, since practically no hypotheses are needed about the original system. The algorithm uses the Singular Values Decomposition (SVD) to analyze dynamic information of the snapshot matrix, which is generated from the data x_k over time t_k.

Mostly, nonlinear dynamical systems are modeled as given by (3), where data measurement is sampled at time t_k.

$$\begin{aligned} x_{k+1} &= F(x_k); k = 1, 2, \ldots, m \\ y_k &= g(x_k) \end{aligned} \tag{3}$$

Where F is the discrete-time flow map of the dynamics and g is the measurement of the system.

We are assuming that all state variables are measured in the most applications of DMD, so that: $y_k = x_k$. The DMD can generate for the system (3), the following global linear dynamic model:

$$x_{k+1} = Ax_k \tag{4}$$

The solution of (4) is given by:

$$x_k = \Phi \Lambda^k b \tag{5}$$

Where Φ and Λ are eigenvectors and eigenvalues of the matrix A respectively, b are coefficients of the initial condition x_1 in the eigenvector basis, so that $x_1 = \Phi b$, (for more details, the reader is referred to [10]). The DMD algorithm produces the reduced eigen-decomposition (5) of the matrix A so the least-square (6), should be minimized for $k = 1, 2, 3 \ldots m - 1$.

$$\|x_{k+1} - Ax_k\|_2 \tag{6}$$

We can arrange the m snapshots in two big data matrices X and X' given by (7) and (8) respectively, where X' is just the shift of X in time by one sample.

$$X = \begin{bmatrix} | & | & | & & | \\ x_1 & x_2 & x_3 & \ldots & x_{m-1} \\ | & | & | & & | \end{bmatrix} \tag{7}$$

$$X' = \begin{bmatrix} | & | & & | \\ x_2 & x_3 & \ldots & x_m \\ | & | & & | \end{bmatrix} \tag{8}$$

Data of (8) are related to data of (7) as follows:

$$X' \approx AX \tag{9}$$

So, the matrix A is given by:

$$A \approx X'X^{\dagger} \tag{10}$$

Where † is the Moore-Penrose pseudo-inverse. The solution (10) should minimize the error given by:

$$\|X' - AX\|_F \tag{11}$$

Where $\|.\|_F$ is the Frobenius norm. When we are dealing with large scale and high dimensional systems as the ADM1, the matrix A might be ungainly to analyze directly, so the DMD algorithm generates a small low rank matrix, $\tilde{A}$ defined as the reduced eigen-decomposition of the matrix A in terms of the Proper Orthogonal Decomposition (POD) projection [11]. The DMD algorithm follows the steps given thereafter [8, 9]:

1. The SVD of the data matrix X:

$$X \approx U\Sigma V^* \tag{12}$$

U are the POD modes, V are the right singular vectors, Σ is the singular values matrix.

2. The A matrix can be calculated from (10) as follows:

$$A = X'V\Sigma^{-1}U^* \tag{13}$$

Where $V\Sigma^{-1}U^* = X^{\dagger}$.
Often, A is very hard to compute, a reduced matrix $\tilde{A}$ is calculated as follows:

$$\tilde{A} = U^*AU = U^*X'V\Sigma^{-1} \tag{14}$$

Thus, we have a low-dimensional linear model of the dynamical system on POD coordinates given by:

$$\tilde{x}_{k+1} = \tilde{A}\tilde{x}_k \tag{15}$$

To reconstruct the high-dimensional state x_k, we can use the formula:

$$x_k = U\tilde{x}_k$$

3. The eigen-decompositon of the matrix $\tilde{A}$ is calculated as follows:

$$\tilde{A}W = W\Lambda \tag{16}$$

Where W and Λ are the eigenvectors and the eigenvalues of the matrix $\tilde{A}$ respectively.

4. Finally, the DMD modes are given by the columns of the matrix Φ:

$$\Phi = X'V\Sigma^{-1}W. \tag{17}$$

We can use the formula below to predict states on a small horizon in the future by running the eigenvalues Λ^t forward in time with the help of DMD modes (Φ) and their amplitudes (b_0):

$$\tilde{x}(k\Delta t) = \Phi\Lambda^t b_0$$

4. Result and discussion

In this section, the simulator BSM2 is running in MATLAB as a virtual process of AD, in order to generate snapshots of data, over a simulation period of 180 days. Since ADM1 has 35 states variables, the snapshot of data contains 35 elements. The sampling time is taken equal to 1 day, so we have finally 180 measurements available for the DMD algorithm. Data matrices are represented as follows by (18),(19) and (20):

$$x_k = \begin{bmatrix} x(x_1, t_k) \\ x(x_2, t_k) \\ . \\ . \\ . \\ x(x_{35}, t_k) \end{bmatrix} \tag{18}$$

$$X = \begin{bmatrix} | & | & | & & | \\ x_1 & x_2 & x_3 & ... & x_{180-1} \\ | & | & | & & | \end{bmatrix} \tag{19}$$

$$X' = \begin{bmatrix} | & | & & | \\ x_2 & x_3 & ... & x_{180} \\ | & | & & | \end{bmatrix} \tag{20}$$

Each column x_k , of the matrix X represents data measurement of 35 variables of ADM1 model at time t_k, $k = 1...179$ (no data for t_{180}). So, size of X is (35*179). Using MATLAB, we applied the DMD algorithm proposed in [8]. After applying the SVD decomposition to our data matrix X, we inspect the sigma matrix Σ given in Table.1 which, contains singular values of the system ADM1. Now, we must keep only the singular values, which correspond to the wanted reduced order of the global linear model. The remained singular values must be truncated, because they correspond to the dynamics which are not dominant for the global system behavior. We decided to keep only 7 modes as illustrated in Table.1 by red color.

σ_i	1	2	3	4	5	6	7	8	9	...	35
1	343.3	0	0	0	0	0	0	0	0	⋯	0
2	0	16.9	0	0	0	0	0	0	0	⋯	0
3	0	0	1.29	0	0	0	0	0	0	⋯	0
4	0	0	0	0.42	0	0	0	0	0	⋯	0
5	0	0	0	0	0.07	0	0	0	0	⋯	0
6	0	0	0	0	0	0.015	0	0	0	⋯	0
7	0	0	0	0	0	0	0.006	0	0	⋯	0
8	0	0	0	0	0	0	0	0.0025	0	⋯	0
9	0	0	0	0	0	0	0	0	0.0017	⋯	0
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋱	0
35	0	0	0	0	0	0	0	0	0	0	0

Table 1 – The matrix Sigma Σ, where singular values are reported in the diagonal and, where the 7^{th} order is the truncation target.

The good advantage of DMD is that we can get a *linear global model* with the ability to choose the linear order approximation that we want. Thanks to the DMD method, the ADM1 model is reduced from 35 states to only 7 states, which are corresponding to dominant dynamics of the AD process. To check that we have rightly chosen the dominant modes in the reduced linear model, we recovered the original data matrix X of the ADM1 model over 180 days (six months of experiment). For illustration of the usefulness of the method, we represent on Figures 3, 4, 5 and 6, data of only four original state variables of ADM1, compared to data which are recovered from the reduced model, using the DMD algorithm. Comparison was done for the first six months (0...180 days), where measurements were taken and, for the latest six months (181...360 days) where no data are available. These preliminary results are very satisfying (for other variables, we have got good result,too). The reduced linear model, can be used for process control purposes. This task will be one of our perspectives, when applying DMD with control.

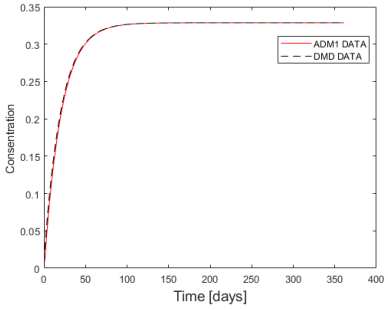


Figure 3 – Concentration of Soluble Inert S_I

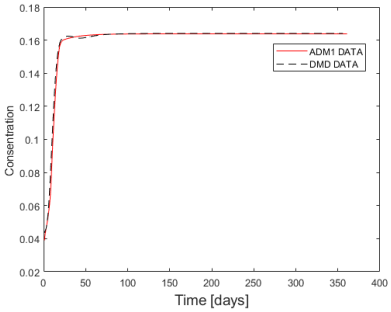


Figure 4 – Concentration of Soluble Inorganic Carbon S_{IC}

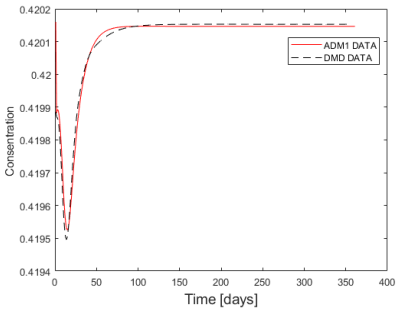


Figure 5 – Concentration of Particulate Sugar X_{su}

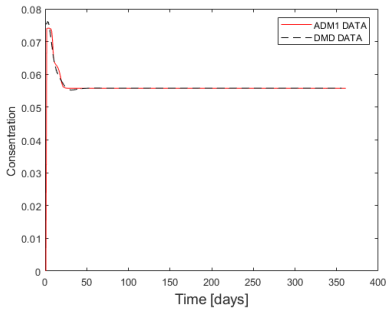


Figure 6 – Concentration of Soluble Methane S_{ch_4}

5. Conclusion

In this paper, a dimensionality reduction method called DMD was presented and applied to deduce a simple linear model from the complex system ADM1 of 35 state vari-

ables. A global linear reduced model was obtained with only 7 state variables, which correspond to the dominant dynamics of the ADM1. Conversely, initial state variables of ADM1 were recovered with the help of the solution from the linear reduced model. Perspectives of this work include i) using the DMD method to elaborate control laws for the process, based on its simple linear model and ii) estimate future states.

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