Towards a systematic approach to reduce complex bioprocess models – Application to the ADM1

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Abstract— **A mathematical reduction method named Homotopy is applied to the Anaerobic Digestion Model No. 1 or ADM1, cf. (Batstone et al., 2002), a complex model of bioprocess describing the anaerobic digestion. Because we are interested in what happens on small timescales, the proposed method neglects the slow dynamics keeping only the fastest ones in using the technique of eigenvalue-state association. This transformation is described by the Homotopy matrix H. Simulations show that the reduced model behaves globally like the initial model at steady states. This approach is confronted with the reduction method using balancing of empirical gramians, an approach that ensures the same input-output behaviour of the reduced model with regard to the original one**.

I. *INTRODUCTION*

In 2002, the IWA Task Group published the Anaerobic Digestion Model No. 1 describing the anaerobic degradation, by different functional microbial species, of complex substrates into intermediate metabolites (notably Volatile Fatty Acids or VFA) and then to gaseous methane (Batstone et al., 2002). This model considers the degradation of the organic matter from its most complex, i.e. the composite organics to its simplest forms, i.e. the gaseous degradation products: carbon dioxide (CO_2), methane (CH_4) and hydrogen (H_2). It involves 35 state variables where the growth kinetics of the biomasses are expressed by Monod type functions while the decay kinetics are first order equations.

In the literature, few works have been done on developing reduced models for controlling complex bioprocesses. For the anaerobic digestion, the model proposed by Bernard et al. (2001) (AM2) is by far one of the most interesting one notably because it has been precisely developed within a framework of a research program dedicated to the control of bioprocesses. This model describes the dynamics of two important substrates of the anaerobic digestion: the complex organic matter (expressed as the Chemical Oxygen Demand or COD) and the VFA. Thus, it simplifies the process to a system of only six state equations. Bernard et al., (2005) proposed another model even simpler than the AM2, named AMH1 which considers only one biomass and two state equations.

De Gracia et al. (2006) proposed a methodology based on the definition of the model components throughout elementary mass fractions and COD estimation. In the works of Rodriguez et al. (2008), the Principal Component Analysis technique was used. Gali et al. (2009) proposed a modified version of the ADM1 based on the model developed by De Gracia et al. (2006) cited above, for the simulation of anaerobic digesters fed on agricultural wastes.

On the one hand, excluding the AM2, these reduced models have rather been obtained within the framework of specific applications of the ADM1. On the other hand, the AM2 describes only the dynamics of aggregated variables such as the COD or the VFA while the ADM1 presents the advantage of using a more detailed matter fractionation.

The idea of the present work is to propose a reduced ADM1 independently of the application for which the use of the ADM1 is intended. The validity of the obtained model will be evaluated around a functioning point.

The first approach is based on a mathematical reduction method named "Homotopy" so as to see if the reduced model can be sufficiently structured with regard to the original ADM1 while approaching the predictions of the latter. In other words, this method aims at evaluating to what extent the ADM1 can be reduced without loss of its structure. The second approach is based on the reduction using balancing of empirical gramians.

The paper is organized as follows: In the first part, we bring simplifications to the kinetics equations and components of the ADM1.Then, we express the reduced model by simplifying the slow dynamics of the model in applying the Homotopy method based on the eigenvalue-state association. This choice of simplifying the slow dynamics is due to the fact that the ADM1 is a dynamic system including different scales of time where the slow dynamics can have time constants of several months, i.e., they reach the steady state after a long time. It is then more interesting to focus on the fast dynamics only, i.e., the ones that rapidly reached the steady state. In the next section, the reduced model obtained is studied at steady state and compared with the ADM1.

The second part of the work deals with the model reduction using balancing of empirical gramians. Moore (1981) introduced balancing with the aim of using it as a tool for model reduction. The idea is that the singular values of the controllability gramian correspond to the amount of energy that has to be put in the system in order to move the

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corresponding states. For the observability gramian, its singular values refer to the energy that is generated by the corresponding states. The use of this second approach can ensure the same input-output behaviour of the reduced model with regard to the original model.

II. REDUCTION USING THE HOMOTOPY METHOD

A. Model reduction

The ADM1 has been applied to many types of digesters, fed with various types of organic matters and working under a wide range of operational conditions. In that regard, its reduction must not affect the model structure - the way the different model components (inputs, states, outputs) are linked and interact - and its abilities to well reproduce and simulate its main components. Usually, model reduction refers as:

- Model simplification: It is a technique which reduces the complexity of the expressions in the model equations while keeping the number of equations of the original model. In general, this is not sufficient to lead to the model reduction in itself;
- Order model reduction: In systems theory, model reduction consists in applying a technique which implies a reduction of the number of the differential equations of the model.

Because a number of simplifications are used before the homotopy method is applied, these two approaches are described in more details in the following sections.

B. Simplification of the kinetics equations

An example of kinetics simplification is the approximation of the Monod growth rate expressions with linear functions, that is, the use of first order reactions for low substrate concentrations and a zero order reaction for high substrate concentrations as proposed in (Blackman, 1905). From a mathematical point of view, this approximation can be formalized as:

$$\mu(S) = \begin{cases} \frac{\mu_{max}}{K_S} S \ \ if\ S \leq K_S \\ \mu_{max} \ \ if\ \ S > K_S \end{cases} \qquad (1)$$

where μ_{max} is the maximum growth rate (1/day) and K_S is the half-saturation constant (gCOD/L). S represents the substrate (gCOD/L) and μ(S) the growth rate (1/day). Furthermore, some authors consider that the reactions are simply of first order with regard to the substrate when the process is operated such that the substrate concentration is always smaller than the affinity constant K_S (Julien, 1997). This approximation will be used for the model reduction in the present article.

C. Simplification of components

Biochemical equations are the core of any model describing a biological system. Assuming it is enough to suit the modeller's objectives and it is theoretically possible to represent an anaerobic system using only these equations [1], that is, to neglect all chemical or physicochemical phenomena. Furthermore, state variables whose dynamics are uncoupled from other components and that are not fundamental for the description of the digester behaviour can be removed from the dynamical system. This is the case of the soluble inert S_I and particulate inert X_I components which are not modified by any of the biochemical processes described in the model.

D. Formulation of the reduced model

1) Simplification of the slow dynamics of the ADM1: First of all, it should be noted that the simplifications cited above were applied to the ADM1 before the simplification of the slow dynamics, that is to say: first order kinetics were used to describe the growth kinetics and substrates uptake instead of the original Monod terms and the state variables S_I and X_I have been removed from the system. These simplifications lead to a system of 33 states.

The technique used in this work for the model reduction is the eigenvalue-state association. Eigenvalues define dynamical properties of linear models and provide fundamental information on the transient response of a system. If the eigenvalues can be bounded to the different model states, then the dynamics of each state can be quantified.

The mathematical method of Homotopy has been initially proposed by De Carlo and Saeks (1979) and Wasynczuk and De Carlo (1981) and was then refined by Robertson (1992). This method implies starting with a system in which the relation eigenvalues-states is obvious such as a decoupled system or a diagonalised matrix A. Later on, this is transformed to a real system by setting out the eigenvalues. The transformation is described by the equation (2).

$$H(r) = (1-r).A_D + r.A \qquad 0 \leq r \leq 1 \qquad (2)$$

where H is the homotopy matrix; A_D is the matrix representing the decoupled equations (diagonal of A); A is the matrix of the linearized model and r is a parameter that allows to obtain a linear progression from the decoupled system to the coupled one. The homotopy matrix H is obtained in proceeding from the decoupled system by varying r from 0 to 1 (in a monotone way), the eigenvalues of H being calculated for each value of r. Thus, the variation of the eigenvalues when r varies from 0 to 1 gives an information on the degree of coupling of the system variables.

In order to apply this method to the ADM1, we assume that the anaerobic digestion takes place in a CSTR (Continuous-flow Stirred Tank Reactor). The steady state input variable and initial conditions values were also those proposed by Rosen and Jeppsson, (2006). Stoichiometric and kinetic parameters were set to their default values which are appropriate to describe the anaerobic digestion of waste activated sludge under mesophilic conditions.

The homotopy method is then applied to a stable equilibrium point of the differential system (composed of thirty five differential equations). It is assumed that the system admits at least one equilibrium point locally asymptotically stable (the real parts of the eigenvalues are strictly negative). For these calculations, the Matlab version 7.2 was used to solve the non linear differential equations system and to calculate the Jacobian of the linearized system around the steady state, and its corresponding diagonal matrix, which are necessary for the calculation of the homotopy matrix H. Then, we can draw the eigenvalues of H as a function of r.

In fact, the aim of the homotopy method is to associate – around a steady state – to each state variable a unique eigenvalue of the linearized system. To do so, we "sweep" r from 0 to 1 to know which eigenvalue of the linearized system we should associate to which state. Thus, and as we will see later, we do not need to study the behaviour (transients) of the resulting model because we will only compare the states at steady state.

2) Simulation results: The results obtained by applying the homotopy method are summarised in the Table 1. It should be noted that the results are only related to the real parts of the eigenvalues, and thus to their equivalence in time constants.

First of all, the soluble components associated to sugars, amino acids, fatty acids, valerate, butyrate and propionate (S_{su}, S_{aa}, S_{fa}, S_{va}, S_{bu}, S_{pro}) present high eigenvalues. Furthermore, the components S_{fa}, S_{va}, S_{bu}, S_{pro} have the real parts of their associated eigenvalues converging to the same values. The dynamic of all the other components are represented by weak eigenvalues, that is to say they have high time constants $\tau_i = -1/\lambda_i$, which means that these components are slow variables for the ADM1.

In order to give a more "physical" sense to these results, it is convenient to "transform" the eigenvalues in their equivalent "time constants" and to interpret these results at the light of the physical meaning of the time constant of a simple linear model.

The Table 1 shows the eigenvalues and the time constants (τ) for each state at the equilibrium point chosen for the study. This table summarizes the information coming from the eigenvalue-state association technique.

3) Expression of the reduced model: The state variables are classified, on a time-constant basis, in two groups:

- The fast states represented in the upper part of the Table 1 and characterized by time constants running from less than one second to less than two minutes;
- Slow states represented in the second part of the table and characterized by time constants running from about two hours to several days.

Applying previous simplifications and including the fact that inhibition terms in the kinetic equations were omitted, the differential system is now reduced to six equations represented by the following state variables: S_{su}, S_{aa}, S_{fa}, S_{va}, S_{bu}, S_{pro} other variables being considered as constants in the time scale of interest.

The model is then described by the following system:

$$\frac{dS_{su}}{dt} = D.\left(S_{su,in} - S_{su}\right) + \eta_6 + \left(1 - f_{fa,li}\right).\eta_8 - \eta_1.S_{su} \tag{3.1}$$

$$\frac{dS_{aa}}{dt} = D.\left(S_{aa,in} - S_{aa}\right) + \eta_7 - \eta_2.S_{aa} \tag{3.2}$$

$$\frac{dS_{fa}}{dt} = D.\left(S_{fa,in} - S_{fa}\right) + f_{fa,li}.\eta_8 - \eta_3.S_{fa} \tag{3.3}$$

$$\frac{dS_{va}}{dt} = D.\left(S_{va,in} - S_{va}\right) + \eta_2.(1 - Y_{aa}).f_{va,aa}.S_{aa} - \eta_4.S_{va} \tag{3.4}$$

$$\frac{dS_{bu}}{dt} = D.\left(S_{bu,in} - S_{bu}\right) + \eta_1.(1 - Y_{su}).f_{bu,su}.S_{su} + \eta_2.(1 - Y_{aa}).f_{bu,aa}.S_{aa} - \eta_4.S_{bu} \tag{3.5}$$

$$\frac{dS_{pro}}{dt} = D.\left(S_{pro,in} - S_{pro}\right) + \eta_1.(1 - Y_{su}).f_{pro,su}.S_{su} + \eta_2.(1 - Y_{aa}).f_{pro,aa}.S_{aa} + 0{,}54.\eta_4.(1 - Y_{c4}).S_{va} - \eta_5.S_{pro} \tag{3.6}$$

where D (1/day) represents the dilution rate (which is defined as the ratio between the influent flow rate and the liquid working volume of the bioreactor: q_{in}/V_l) and $S_{su,in}$ (kgCOD/m³), $S_{aa,in}$ (kgCOD/m³), $S_{fa,in}$ (kgCOD/m³), $S_{va,in}$ (kgCOD/m³), $S_{bu,in}$ (kgCOD/m³), $S_{pro,in}$ (kgCOD/m³), represent the concentrations of S_{su}, S_{aa}, S_{fa}, S_{va}, S_{bu} and S_{pro} respectively in the influent and where the specific parameters η_1 (1/d), η_2 (1/d), η_3 (1/d), η_4 (1/d), η_5 (1/d)), η_6 (kgCOD/m³/d), η_7 (kgCOD/m³/d) and η_8 (kgCOD/m³/d) are defined according to state variables and parameters of ADM1 model by:

$$\eta_1 = \frac{k_{m,su}}{K_{s,su}}.X_{su} \tag{4}$$

$$\eta_2 = \frac{k_{m,aa}}{K_{s,aa}}.X_{aa} \tag{5}$$

$$\eta_3 = \frac{k_{m,fa}}{K_{s,fa}}.X_{fa} \tag{6}$$

$$\eta_4 = \frac{1}{2}.\frac{k_{m,c4}}{K_{s,c4}}.X_{c4} \tag{7}$$

$$\eta_5 = \frac{k_{m,pro}}{K_{s,pro}}.X_{pro} \tag{8}$$

$$\eta_6 = k_{hyd,ch}.X_{ch} \tag{9}$$

$$\eta_7 = k_{hyd,pr}.X_{pr} \tag{10}$$

$$\eta_8 = k_{hyd,li}.X_{li} \tag{11}$$

E. Study of the reduced model at steady state

1) Operational conditions

As stated before, the case study is a CSTR anaerobic digester fed on waste activated sludge operating under mesophilic temperature and typical loading conditions. More specifically, the following operational and input data were assumed:

- Hydraulic retention time (HRT): 20 days
- Sludge retention time (SRT): 20 days
- Influent concentrations of all relevant components: as suggested by Rosen et al., 2006.

Table 1 – Eigenvalue (real part) and time constant association

State Variables	|Eigenvalues| (1/Day)	τ (h)
Ssu	***1,27E+03***	***3,28E-05***
Saa	***1,84E+01***	***2,27E-03***
Sfa	***2,01E+00***	***2,07E-02***
Sva	***1,76E+00***	***2,37E-02***
Sbu	***1,60E+00***	***2,60E-02***

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Spro	***1,53E+00***	***2,72E-02***
Sac	2,17E-02	1,92E+00
Sh2	6,53E-03	6,38E+00
Sch4	3,59E-03	1,16E+01
Sic	2,27E-03	1,83E+01
Sin	9,43E-04	4,42E+01
Xc	6,12E-04	6,80E+01
Xch	4,73E-04	8,80E+01
Xpr	2,92E-04	1,43E+02
Xsu	2,51E-04	1,66E+02
Xli	2,50E-04	1,67E+02
Xaa	2,07E-04	2,02E+02
Xc4	1,16E-04	3,58E+02
Xh2	1,16E-04	3,58E+02
Scat	1,16E-04	3,58E+02
Xfa	4,22E-05	9,88E+02
Xpro	1,62E-05	2,57E+03
Xac	6,39E-06	6,52E+03
Sbum	8,13E-07	5,12E+04
Sprom	8,11E-07	5,14E+04
Sacm	8,11E-07	5,14E+04
Shco3	8,10E-07	5,14E+04
Snh3	8,10E-07	5,14E+04
Sgash2	8,10E-07	5,14E+04
Svam	7,88E-07	5,29E+04
San	5,79E-07	7,20E+04
Sgasch4	5,79E-07	7,20E+04
Sgasco2	5,79E-07	7,20E+04

Simulations were performed by using DYMOLA (DYnamic MOdeling LAboratory), a modeling and simulation platform based on the Modelica language and that is especially efficient in the simulation of large ODE systems as the ADM1.

2) Comparison between the ADM1 and the reduced model: Simulations were performed under constant operational and loading conditions, to compare the values assumed by the state variables at steady state as predicted by the ADM1 and by the reduced model (Table 2).

At a first glance it appears that the state variables of the reduced model behave globally – at least qualitatively - as the original ones (trajectories of the ADM1).

Table 2 – Steady state values reached by the two models

States variables	Units	ADM1	Reduced model	|Relative error| (%)
Ssu	gCOD/L	0,0119	0,0117	1,68
Saa	gCOD/L	0,0053	0,0052	1,89
Sfa	gCOD/L	0,0986	0,0758	23,12
Sva	gCOD/L	0,0116	0,0100	13,79
Sbu	gCOD/L	0,0132	0,0129	2,27
Spro	gCOD/L	0,0158	0,0128	18,99

F. Sensitivity study

It has been considered by Batstone et al., 2002 that a number of states of the ADM1 are particularly sensitive to several parameters, i.e., they present a significant sensitivity under steady state conditions with respect to some model parameters. It is thus important to evaluate the sensitivity of the states of the reduced model with respect to these parameters. Different approaches are possible to determine the functions of sensitivity $\partial y_j/\partial p_i$. Practically, if we consider a deviation Δp_i for the parameter p_i, we can estimate the sensitivity of a state with respect to the considered parameter. An index of sensitivity has been proposed by Dochain et Vanrolleghem (2001) as follows:

$$\delta_{ij} = \frac{p_i}{y_j(p_i)}.\frac{y_j(p_i+\Delta \mathrm{p_i})-\mathrm{y_j(p_i)}}{\Delta \mathrm{p_i}}.100. \qquad (12)$$

For each parameter p_i, an absolute variation Δp_i of 20% of the default value was then applied.

Table 3 reports the results of the ADM1 and reduced model sensitivities study with regard to the different model parameters. As we can see, the sensitive parameters are the same in the ADM1 and reduced model. Moreover, the sensitivities of the states with regard to the parameters are preserved in the reduced model.

From these simulations we can consider that the ADM1 and the reduced model have the same behaviour at steady state around the considered equilibrium point. However, it must be stressed that the reduced model is available in the absence of perturbations and control; this, because we cannot ensure that the perturbations and the control do not modify the eigenvalue –state association.

Thus, this approach is interesting for the study of, for example, the qualitative behaviour in open loop but for the control we may prefer an approach which can preserves the input-output behaviour. This is explained in the next part of this work with the second approach.

III. REDUCTION USING BALANCING OF EMPIRICAL GRAMIANS

A. Reduction of the linear dynamic system

The ADM1 system is a nonlinear control-affine system with a representation of the following form:

$$\begin{cases} \dot{x} = f\big(x(t)\big) + g\big(x(t)\big)u(t) \\ \qquad y(t) = h(x(t)) \end{cases} \qquad (13)$$

where f, g and h are functions of class C^{∞}.

For the linear control system reduction, the linearization of the ADM1 system was carried out around an operating point corresponding to the steady state conditions of a CSTR anaerobic digester and this led to the LTI system of the form:

$$\begin{cases} \dot{x} = Ax(t) + Bu(t) \\ y(t) = Cx(t) \end{cases} \quad (14)$$

with $A \in \mathbb{R}^{35x35}$; $B \in \mathbb{R}^{35x1}$and $C \in \mathbb{R}^{1x35}$

B. Balancing of the linear system

Checking the controllability and the observability of the system it appears that the system has one uncontrollable mode and it is observable, furthermore, the matrix A is Hurwitz.

We define the controllability and the observability gramians respectively as:

$$W_C = \int_0^\infty e^{At} B B^T e^{A^T t} dt, \quad (15)$$

$$W_O = \int_0^\infty e^{A^T t} C^T C e^{At} dt. \quad (16)$$

It is well known that the two gramians satisfy the Lyapunov equations given by: [15]

$$A W_C + W_C A^T = -B B^T \quad (17)$$

$$A^T W_O + W_O A = -C^T C \quad (18)$$

In our case it should be noticed that, the two gramians are not equal. This result was expected because of the uncontrollable mode of the system. Thus, we should find new coordinates of the system such that:

$$\widetilde{W}_C = \widetilde{W}_O = \Sigma = \begin{bmatrix} \sigma_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_n \end{bmatrix} \quad (19)$$

with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ are the Hankel singular values.

A system whose gramians verify the above equality is called balanced and the transformed gramians are given by:

$$\widetilde{W}_C = T W_C T^T \quad (20)$$

$$\widetilde{W}_O = (T^{-1})^T W_O T^{-1} \quad (21)$$

Furthermore, there exists a transformation $\tilde{x} = Tx$ such that the transformed system given by:

$$\begin{cases} \dot{\tilde{x}} = TAT^{-1}\tilde{x} + TBu \\ y = CT^{-1}\tilde{x} \end{cases} \quad (22)$$

is balanced.

Using the MATLAB software we got the transformed gramians $\widetilde{W}_C$ and $\widetilde{W}_O$, and the linear transformation matrix T with $T \in \mathbb{R}^{35x35}$. This way, we obtain a balanced realization of our linear system.

C. Truncation of the balanced realization

If a linear system is in a balanced form, the Hankel singular values provide a measure for the importance of the states. We will use this property in order to reduce the model.

For model reduction, the states that contribute very little to the input-output behaviour can be removed. As shown in Figure 1, weak or least controllable and observable states are quantified by zero and close to zero Hankel singular values from the order 5.

But before making the choice of the reduced order model, one must define the error bound at which maximum errors in model order reduction is quantified. For a kth reduced order model, this error bound is computed by:

$$\|G(s) - G(s)_{red}\|_\infty \leq 2\sum_{i=k+1}^{n} \sigma_i \quad (23)$$

where σ_i are the Hankel singular values.

Table 3 – Results of the sensitivity study of ADM1 and reduced model with regards to the joint parameters: 1 = δ_{ij} < 30%; 2 = 30% ≤ δ_{ij} ≤ 60%; 3 = δ_{ij} > 60%

	$k_{m,su}$	$K_{s,su}$	$k_{m,aa}$	$K_{s,aa}$	$k_{m,fa}$	$K_{s,fa}$	$k_{m,c4}$	$K_{s,c4}$	$k_{m,pro}$	$K_{s,pro}$	$k_{hyd,ch}$	$k_{hyd,pr}$	$k_{hyd,li}$
Ssu (ADM1)	3	3									3		1
Ssu (reduced)	3	3									3		1
Saa (ADM1)			3	3								1	
Saa (reduced)			3	3								1	
Sfa (ADM1)					3	3							1
Sfa (reduced)					3	3							1
Sva (ADM1)			1	1			3	3					
Sva (reduced)			1	1			3	3					
Sbu (ADM1)	1	1	1	3			3	3					
Sbu (reduced)	1	1	1	3			3	3					
Spro (ADM1)	1	1	1	1			1	1	3	3			
Spro (reduced)	1	1	1	1			1	1	3	3			

Table 4 shows errors bounds for some different orders. It seems that the order 14 is a reasonable choice leading to a reduced model represented by a reasonable error bound.

Figure 2 compares the two systems using Bode plots. As can be seen, the two systems behave very similarly at low frequency, the response of the reduced model provide a good approximation for the real system.

It is not really the case at high frequencies. However, the models are usually chosen to represent a system mostly at low frequencies while the high frequency response is usually less important for controller operation (Skogestad , 1997).

Other important measures for model comparison are the impulse and the step responses. As we can see in Figure 3, there is a good approximation of the reduced model with regard to the original one. The detailed of the reduced system expression is not given here because of lack of space. Our system is now of order 14.

Even if this second approach leads to a reduced model with a greater order than the one obtained with the first approach, this is, first, a consistent reduction compared with the initial 35 states system and secondly, the input-output behaviour is preserved with this last approach.

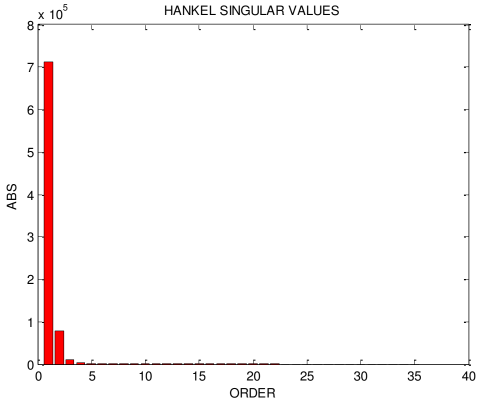

Fig. 1. Hankel singular values of the LTI system

Table 4 - Errors bounds for different orders

Reduced order model	Error bound
16	2.1937e-003
15	1.0759e-002
14	**2.0123e-002**
13	3.1882e-002
12	9.0309e-001
11	5.7522e+000

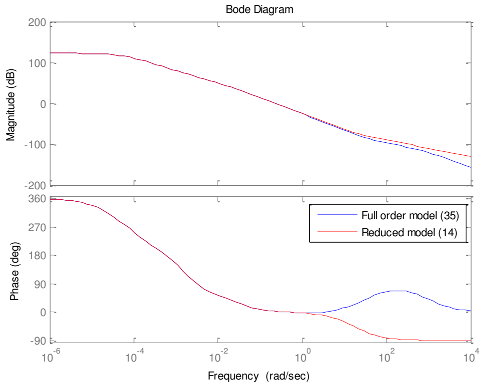

Fig. 2. Bode plot comparison of full order and reduced systems

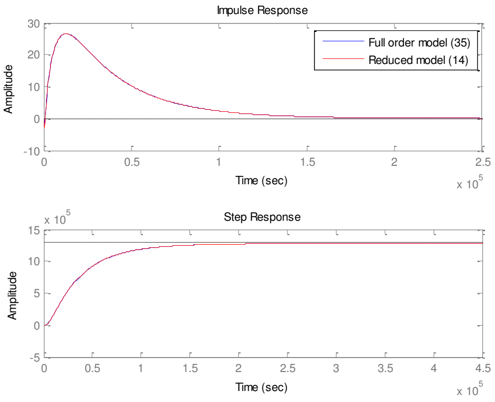

Fig. 3. Impulse and step responses of full order and reduced systems

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