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OBTAINING LINEARIZED DYNAMIC MODELS FROM STEADY-STATE SIMULATIONS

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Resumo: *The stages of design, analysis and optimization of chemical processes are usually based on stationary simulations, since dynamic informations are missing at this stage apart from the difficulty and cost of obtaining dynamic models. Moreover when the dynamic simulation is used to design linear control, linearized models are usually used from sensitivity analysis or by fitting an empirical model. The proposed method is based on a generic framework that relates a dynamic model with its underlying static model. When a static model is developed, the inventory part of the dynamic model (i.e. tank size, diameter and height of tray, and so on) is not included. Therefore, we should include theses information again but not in the static model directly. Instead of that, we use this information as a part of the problem, that is, the information about steady-state is guaranteed and there is no loss of static result. All results described in this paper show that the linearized models by this method are equivalent to those obtained by the dynamic model even with interactions between mass and energy balances.*
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Palavras-chave: *linearized models, static simulations, dynamic models, design and control.*

1. Introduction

The need for cost containment in the chemical industry has introduced a trend towards the realization of highly integrated process, and the validation of design integrity and its practical operability require the simulation of the whole process with use of rigorous models. But the more accurate is the process description, greater the resulting set of equations and more difficult to treat. Moreover the stages of design, analysis and optimization of chemical processes are usually based on steady-state simulations of this process, since dynamic information are usually ignored in this stage, besides the difficulty and cost of obtaining dynamic models. This makes that stationary models of processes are more widespread than dynamic models. However, at later stages of the project, involving, for example the control strategy, a dynamic model of the process is very important. Whereas the benefits of employing computer tools for process design, planning and off-line optimization become evident, and consequently their use in practice widespread, the same is not true for on-line and dynamic simulation. Although this type of model can potentially lead to enormous benefits as well as applications ranging from operator training to dynamic optimization, the cost of developing such model is still inhibiting, at least at a useful degree of realism. In this way, any methodologies that help to bridge the gap between the conceptual design of such tools and their industrial application are greatly welcome.

Usually, alternative designs are judged on economics alone without taking operability into account. This may lead to the elimination of easily-controlled but slightly less economical alternatives in favor of more economical designs which may be extremely difficult to control (Weitz and Lewin, 1996). One appealing possibility with this regard is to use simplified or shortcut dynamic representations based on steady-state models. It is quite common that a stationary model has been developed in some environment that does not support dynamic modeling. In this case, a methodology of making use of this model for the construction of consistent dynamic extension would be very beneficial. In addition, when the dynamic simulation is employed for linear control design, it is generally used to generate linearized models (either from sensitivity analysis or from adjusting models on the base of time responses), which are then used for tuning controller parameters (Bolognese Fernandes and Trierweiler, 2007).

The integration of design and control received much attention in the past years. Weitz and Lewin (1996) describe a simple procedure which can be used to investigate the degree to which a process flowsheet is resilient to external disturbances and the approach involves the derivation of an approximate linear dynamic plant model, generated solely from steady-state flowsheet information and independent of control system design. Methods that allow for the study of input-output controllability issues – that is, poles and zeros of the

linearized models, RGA, RPN, and so on (Trierweiler, 2002; Engell et al., 2004) – on the basis of steady-state models could facilitate greatly this kind of analysis, since it is generally carried out around an equilibrium state.

The present paper aims at verifying the possibilities for the generation of dynamic models on the basis of steady-state ones. Since the main focus of the paper is on control and dynamic optimization, it is interesting to obtain the linearized models of the process to be studied. In this case, there are two possibilities: directly from dynamic models or combination of the linearized stationary model and the dynamic part of the process.

2. Linearized and Dynamic Models from Static Simulations

The fundamental laws of mass and energy conservation, when applied to a dynamic system, states that the variation rate of mass or energy in a differential volume control is equal to the difference between the rate of mass or energy that enters and leaves the element, plus generation rate of mass or energy. At steady state, the variation rate is neglected and the resulting equations are used to process design. That is, some information about process dynamic are not present in the stationary model.

2. 1. Homogenous Systems

Consider a system constituted by N control volumes containing a single species. The mass balance around each of these elements can be written in vector form as (Elnashaie and Garhyan, 2003):

$$\frac{d\mathbf{M}}{dt} = \mathbf{k} \cdot f_{ss} \tag{1}$$

where $\mathbf{M} = [m_1\ m_2\ \ldots\ m_N]^T$ is the vector of mass and energy holdups, f_{ss} is the steady-state model and $\mathbf{k}$ is a diagonal matrix of common factors that relates the stationary model with mass and energy conservation. A common situation is when we are not interested directly on $\mathbf{M}$, but on a property derived the vector $\mathbf{q}$ (such as level of liquids, gas pressure, temperature, and so on), which will be called here the *state variables of the problem*. These are related to the mass and energy holdups by means of a relation of the form $\mathbf{M} = \mathbf{M}(\mathbf{q})$ In this case the balance can be expressed in terms of the new state variables as

$$\frac{d\mathbf{q}}{dt} = \mathbf{k}\left[\frac{\partial \mathbf{M}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1} f_{ss} \tag{2}$$

In Eq. (2) the term $\partial\mathbf{M}(\mathbf{q})/\partial\mathbf{q}$ represents the variation of conserved property by related states and it's called "mass matrix". The stationary model usually depends on the state variables and, more specifically on control applications, manipulated variables ($\mathbf{u}$). Therefore, the Eq. (2) can be rewritten as

$$\frac{d\mathbf{q}}{dt} = \mathbf{k}\left[\frac{\partial \mathbf{M}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1} f_{ss}(\mathbf{q},\mathbf{u}) \tag{3}$$

In this way the dynamic model is constructed using information from static simulations and additional information about the dynamics of process.

2. 2. Homogenous Reaction Systems

Consider now a single control volume, in which a set of *m* chemical reactions involving *P* species takes place. The dynamic balance is now of the form (Elnashaire and Garhyan, 2003):

$$\frac{d\mathbf{n}}{dt} = \boldsymbol{\Theta}_{in} - \boldsymbol{\Theta}_{out} - \boldsymbol{\nu} \tag{4}$$

where $\mathbf{n} = [n_1\ n_2\ \ldots\ n_P]^T$ are the number of moles of the individual species, $\boldsymbol{\Theta}_{in}$ and $\boldsymbol{\Theta}_{out}$ are the mole flow into and from the system, and $\boldsymbol{\nu}$ are the overall generation/depletion rates due to chemical reaction. These reaction terms are generally written as volumetric rates; moreover, it is also customary to write them in terms of the Law of mass action, that is, as a function of the individual molar concentrations. This makes the concentration $\mathbf{c}$ a more natural state variable, and since $\mathbf{n} = \mathbf{c}V$, the mole balance becomes:

$$\begin{aligned}\frac{d}{dt}(\mathbf{c}\cdot V) &= V\cdot\frac{d\mathbf{c}}{dt} + \mathbf{c}\cdot\frac{dV}{dt} = \\ &\boldsymbol{\Theta}_{in} - \boldsymbol{\Theta}_{out} - \boldsymbol{\nu}(\mathbf{c})\cdot V = \\ &\mathbf{c}_{in}\cdot\Lambda_{in} - \mathbf{c}\cdot\Lambda_{out} + \boldsymbol{\nu}(\mathbf{c})\cdot V = 0\end{aligned} \tag{5}$$

where V is the volume of the reacting mixture and $\Lambda_{in,out}$ are the volumetric in/outflows. Because the system is constituted by a single control volume, it is possible to consider $\boldsymbol{\Theta}_{in}$ as an external input (in case of no feedback loops). Obviously, an extra equation is necessary to account for the variation in the volume, which can be obtained, for example, by an overall mass balance. We can write this extra equation as a relationship similar to Eq. (1), that is:

$$\begin{aligned}\frac{d}{dt}(\boldsymbol{\rho}(\mathbf{c})\cdot V) &= \boldsymbol{\Phi}_{in} - \boldsymbol{\Phi}_{out} \\ &= \boldsymbol{\rho}(\mathbf{c}_{in})\cdot\Lambda_{in} - \boldsymbol{\rho}(\mathbf{c}_{out})\cdot\Lambda_{out}\end{aligned} \tag{6}$$

where $\boldsymbol{\rho}$ is the specific mass of the mixture (which is in general a function of its concentration) and $\boldsymbol{\Phi}_{in}$,out are the overall mass flows into/out of the system.

3. Linearization

Additionally to the construction of dynamic models on the basis of stationary representations, another interesting application of this analysis concerns the Taylor linearization of the Eq. (3), which is of the form:

$$\Delta\overline{\frac{\partial\mathbf{q}}{\partial t}} = \mathbf{A}\cdot\Delta\bar{\mathbf{q}} + \mathbf{B}\cdot\Delta\mathbf{u} \tag{7}$$

where "–" stands for the fact that the linearized states are approximations of $\mathbf{q}$, and the matrices $\mathbf{A}$ and $\mathbf{B}$ are given by:

$$\mathbf{A} = \mathbf{k}\frac{\partial}{\partial \mathbf{q}}\left(\left[\frac{\partial \mathbf{M}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1}\right) f_{ss}(\mathbf{q},\mathbf{u}) + \mathbf{k}\left[\frac{\partial \mathbf{M}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1}\frac{\partial f_{ss}(\mathbf{q},\mathbf{u})}{\partial \mathbf{q}} \quad (8)$$

$$\mathbf{B} = \mathbf{k}\left[\frac{\partial \mathbf{M}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1}\frac{\partial f_{ss}(\mathbf{q},\mathbf{u})}{\partial \mathbf{u}} \quad (9)$$

Particularly for the linearizations corresponding to equilibrium points (steady-states), the dynamic matrix **A** is constituted solely by the product of the inverse of the mass matrix and the gradient of the stationary model with respect to **q** (all evaluated at steady-state), since the first term in Eq. (8) vanishes for any stationary solution of Eq. (3).

There are two ways to obtain the linearized dynamic model: from dynamic model directly or from combination between linearized stationary model and dynamic part of the process. In this way, we can otain the matrices **A** and **B** without need to develop the dynamic model.

Another possibility with this respect is to consider these parameterized models to formulate controlled optimization problems, in which one is interested in finding the best setting (operating point, holdups) in order to achieve good control performance, or to minimize any measure (RGA, non-linearity, and so on) that can be parameterized in terms of the equilibrium points (Bolognese Fernandes and Trierweiler, 2007).

3. Numerical Example

To exemplify the methodology, it will be shown how a dynamic model of the level system shown schematically in Figure (1) can be constructed on the basis of the previous analysis. The plant is constituted by three spherical tanks with different diameters D_i [*cm*] disposed in series. Water flows from tank 1 to tank 3 by gravity at constant temperature and the flows are assumed to be turbulent. The manipulated variable is the inlet flow rate of the first tank, F_0 [cm^3/min]. The state variables (called q in the previous discussion) are the liquid levels L_i [*cm*] in the tanks, i = 1, 2, 3.

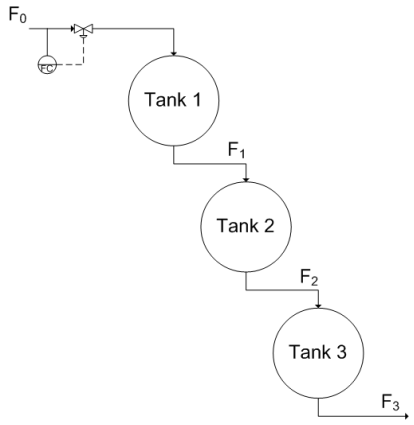

Figure 1. Diagram of the spherical tank system.

The stationary model of the system has written in the implicit form given by Eq. (10) and depends on the state variables as showed in Eq. (11).

$$f_{ss} = \begin{bmatrix} F_0 - F_1 \\ F_1 - F_2 \\ F_2 - F_3 \end{bmatrix} = 0 \quad (10)$$

$$F_i = C_{v,i}\sqrt{L_i} \quad (11)$$

In order to generate a dynamic model on the basis of Eq. (7), as described in Section 2, it is necessary to represent the dependence **M** = **M**(**q**) of the holdup in each compartment with the respective level. Since the tanks are spherical, this relationship is given by

$$m_i = \rho V_i = \rho\frac{\pi}{3}h_i^2\left(\frac{3}{2}D_i - h_i\right) \quad i = 1,2,3 \quad (12)$$

To generate the dynamic model is necessary to get the inverse holdup matrix according to Eq. (3). In this case, we want to evaluate the liquid level in each tank with respect to time. Thus, the vector of state variables is **q** = $[L_1\ L_2\ L_3]^T$ and the inverse holdup matrix is described by Eq. (13):

$$\left[\frac{\partial \mathbf{M}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1} = \begin{bmatrix} \frac{1}{\pi(D_1 - L_1)L_1} & 0 & 0 \\ 0 & \frac{1}{\pi(D_2 - L_2)L_2} & 0 \\ 0 & 0 & \frac{1}{\pi(D_3 - L_3)L_3} \end{bmatrix} \quad (13)$$

The matrix **k** is represented by diag($\rho_1\ \rho_2\ \rho_3$)in this case and it was considered constant for convenience (ρ_1=ρ_2=ρ_3). The dynamic model is represented by Eq. (14).

$$\begin{cases} \frac{dL_1}{dt} = \frac{F_0 - C_{v,1}\sqrt{L_1}}{\pi(D_1 - L_1)L_1} \\ \frac{dL_2}{dt} = \frac{C_{v,1}\sqrt{L_1} - C_{v,2}\sqrt{L_2}}{\pi(D_2 - L_2)L_2} \\ \frac{dL_3}{dt} = \frac{C_{v,2}\sqrt{L_2} - C_{v,3}\sqrt{L_3}}{\pi(D_3 - L_3)L_3} \end{cases} \quad (14)$$

The algebraic equations are decoupled from the state equations, in the sense that they can be solved separately for the L_i and thus the system is not a “true” DAE representation. Observe that the dynamic model is in the form of Eq. (3) and was obtained solely on the basis of Eq. (10), which can be in principle a heuristic steady-state model or a “black-box” function, as compiled routine, for example. The model was compared with the one obtained by the traditional, or direct, approach, that is, by directly writing down the dynamic balances.

An interesting application is to employ sensitivity studies of the steady-state model, coupled with the information given by Eq. (12), in order to determine the Taylor linearizations of the system, as described in Section 3. In order to illustrate this, the three tanks system consist of the characteristics showed in Table 1, and the matrices

A and **B** of three linear models, were obtained by dynamic model, Eq. (15) and compared with matrices obtained by this shortcut method, Eq. (16), at the equilibrium points by the feed flow rate of 7070 cm^3/min and was compared with the values determined by linearization of model.

Tabela 1. Tank's characteristics.

Tank	1	2	3
$D_i\,[cm]$	35	20	25
$C_{v,i}\,[m^{2.5}/min]$	0.0169	0.0183	0.02

$$\mathbf{A}_{\text{model}} = \begin{bmatrix} \frac{1}{2}\frac{C_{v,1}}{\pi(L_1-D_1)L_1^{3/2}} + A_{1,1} & 0 & 0 \\ -\frac{1}{2}\frac{C_{v,1}}{\pi(L_2-D_2)L_2\sqrt{L_1}} & \frac{1}{2}\frac{C_{v,2}}{\pi(L_2-D_2)L_2^{3/2}} + A_{2,2} & 0 \\ 0 & -\frac{1}{2}\frac{C_{v,1}}{\pi(L_3-D_3)L_3\sqrt{L_2}} & \frac{1}{2}\frac{C_{v,3}}{\pi(L_3-D_3)L_3^{3/2}} + A_{3,3} \end{bmatrix} \tag{15}$$

$$\mathbf{A}_{\text{method}} = \begin{bmatrix} \frac{1}{2}\frac{C_{v,1}}{\pi(L_1-D_1)L_1^{3/2}} & 0 & 0 \\ -\frac{1}{2}\frac{C_{v,1}}{\pi(L_2-D_2)L_2\sqrt{L_1}} & \frac{1}{2}\frac{C_{v,2}}{\pi(L_2-D_2)L_2^{3/2}} & 0 \\ 0 & -\frac{1}{2}\frac{C_{v,1}}{\pi(L_3-D_3)L_3\sqrt{L_2}} & \frac{1}{2}\frac{C_{v,3}}{\pi(L_3-D_3)L_3^{3/2}} \end{bmatrix} \tag{16}$$

$$\mathbf{B}_{\text{model}} = \mathbf{B}_{\text{method}} = \begin{bmatrix} -\frac{1}{\pi(L_1+D_1)L_1} & 0 & 0 \end{bmatrix}^T \tag{17}$$

$$A_{i,i} = \frac{F_{i-1} - F_i}{\pi(L_i - D_i)^2 L_i - \pi(L_i - D_i)L_i^2} \tag{18}$$

The matrices **A** obtained by this method and from the dynamic model are equal when $A_{i,i} = 0$, that is, when we perform the linearization around a stationary point. For any desviation from steady-state, the first term of matrix **A** in Eq. (8) is not zero, because $f_{ss}(\mathbf{q},\mathbf{u}) \neq 0$ and it must take into a count or evaluate the new steady-state point.

4. Mass and Energy Systems Coupled

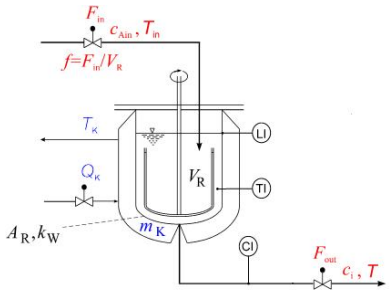

Figure 2. Schematic representantion of the CSTR.

This methodology can also be applied toprocess involving mass and energy balances. For this, we used as an example the Van de Vusse reaction (Trierweiler, 1997), where cyclopentenol (B) is produced from cyclopentadiene (A) and the by-products cyclopentanediol (C) and dicyclopentadiene (D) are produced in unwanted side and consecutive reations,

$$\begin{aligned} A &\xrightarrow{k_1} B \xrightarrow{k_2} C \\ 2A &\xrightarrow{k_3} D \end{aligned} \tag{19}$$

is carried out in a CSTR. Figure (2) shows the reactor schematically.

Under the assumption of constant density the steady-state model can be described by the following equations that are derived from mass and energy balances for the reactor and the cooling jacket:

$$f_{ss} = \begin{bmatrix} F_{in}C_{Ain} - F_{out}C_A - V_R(r_1 + r_3) \\ -F_{out}C_B + V_R(r_1 - r_2) \\ \rho c_P(F_{in}T_{in} - F_{out}T) + KwAr(T_k - T) + Q \\ Q_k + KwAr(T - T_k) \\ \rho(F_{in} - F_{out}) \end{bmatrix} \tag{20}$$

where Q is the term referring to energy rate generated by the raction:

$$Q = -\left(r_1 \Delta H_1 + r_2 \Delta H_2 + r_3 \Delta H_3\right) \tag{21}$$

The raction rate (r_1, r_2 *and* r_3) and the specific reaction rate are assumed to depend on the temperature via Arrhenius equation

$$r_j = k_{j,0} \exp\left(\frac{E_j}{T + 273{,}15}\right)\begin{bmatrix} C_A \\ C_B \\ C_A^2 \end{bmatrix} \tag{22}$$

$$j = 1,2,3$$

The state variables of this problem are C_A, C_B, T, T_k, V_R, respectively, and the mass and energy holdup is given by as described in Section 2.1.

$$\mathbf{M}(\mathbf{q}) = \begin{bmatrix} C_A V_R \\ C_B V_R \\ V_R \rho c_P T \\ m_k c_{Pk} T_k \\ \rho V_R \end{bmatrix} \tag{23}$$

In this case, the holdup matrix, Eq. (24) is not a diagonal matrix, but a matrix with elements outside the main diagonal. This occurs due to combination of state variables in mass and energy holdup. According to Section 3 we can obtain the linearized model such as described by Eqs. (8) and (9). The results of linearized model obtained by this methodology were compared to linearized model from dynamic model according to Trierweiler (1997).

$$\left[\frac{\partial \mathbf{M}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1} = \begin{bmatrix} \frac{1}{V_R} & 0 & 0 & 0 & -\frac{C_A}{\rho V_R} \\ 0 & \frac{1}{V_R} & 0 & 0 & -\frac{C_B}{\rho V_R} \\ 0 & 0 & \frac{1}{\rho c_P V_R} & 0 & -\frac{T}{\rho V_R} \\ 0 & 0 & 0 & \frac{1}{m_k c_{Pk}} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\rho} \end{bmatrix} \tag{24}$$

The reactor design was developed with the set of paraters showed in Table (2) and (3):

Table 2. Chemical kinetic parameters for the Arrehnius equation.

Reaction	Collision factor $k_{i,0}$	Unit of $k_{i,0}$	Activation Energie E_i	Reaction Enthalpy
$r_1=k_1(T)C_A$	$1.287\text{x}10^{12}$	1/h	-9758.3 *K*	4.2 *kJ/mol*
$r_2=k_2(T)C_B$	$1.287\text{x}10^{12}$	1/h	-9758.3 *K*	-11.0 *kJ/mol*
$r_3=k_3(T)C_A^2$	$9.043\text{x}10^{09}$	l/mol/h	-8560 *K*	-41.8 *kJ/mol*

Table 3. Physico-chemical parameters and reactor dimensions.

Parameter	Symbol	Value	Unit
Density	ρ	0.9342	*kg/l*
Heat capacity	c_p	3.01	kJ/kg/K
Heat transfer coefficient	*Kw*	4032	$kJ/m^2/h/K$
Surface of cooling water	*Ar*	0.215	m^2
Coolant mass	m_k	5.0	*kg*
Heat capacity of coolant	c_{pk}	2.0	kJ/kg/K

The steady-state point was evaluated for the input variables: F_{in} *= 141.9 l/h;* C_{Ain} *= 5.1 mol/l;* T_{in} *= 104.4 K;* Q_k *= -1113.1 kJ/h.* Therefore, the state variables at stationary points are: C_A *= 2.18 mol/l;* C_B *= 1.09 mol/l;* T *= 113.6 K;* T_k *= 112.3 K.* The Figure (3) shows the linearized models by method (lines) and by model (circles) for concentration of (A) and (B). Both results are presented in deviation variables form ($\Delta C_A = C_A - C_{Ass}$ and $\Delta C_B = C_B - C_{Bss}$). The Figure (3a) represents the variation of concentrations from a unit step in C_{Ain} and in Figure (3b) the unit step was on T_{in}.

In view of results we can say that the methodology described is valid and can be used to obtain the linearized models without obtaining the dynamic model. Only results from stationary and information about the process dynamic are necessary. This example shows that the methodology can be used in conjunction with mass and energy balance.

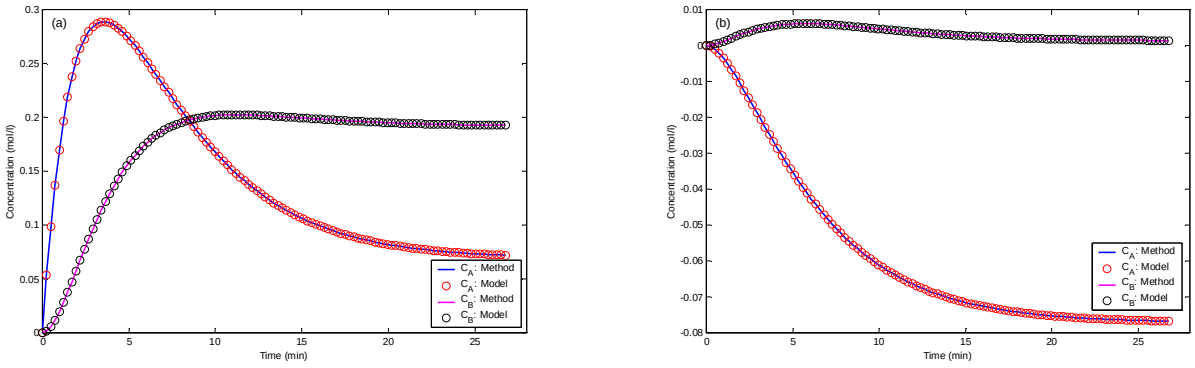

Figure 3. Linearized model from the proposed method (–) and from model (O) with a unit step in C_{Ain} (a) and in T_{in} (b).

4. Conclusions

This paper showed some possibilities of exploiting steady-state information in order to construct linearized dynamic models, as well as the necessary extra information to produce them. The analysis was restricted to lumped models, although, at least in the last situation, extensions seem to be straightforward. Through this methodology, we can model a dynamic system from an existing stationary model. The application of this methodology in obtaining dynamic and linearized models from stationary model is demostrated, as discussed in the examples presented. The examples were chosen to demonstrate that this methodology is valid in cases where there is integration between the states variables. Thus it has shown that the linearized model can be obtained by deriving the stationary model and, after that, including dynamic information of the process. Note also that the linearization of dynamic models can be obtained at an intermediate step of the methodology, without obtaining the dynamic model firstly. As demonstrated with the examples, the technique can be applied to different types of systems (reaction systems, heat exchangers, column distillation, and on) with or without mass and energy coupling.

This proposed approach can also be extended and combined with different tools. For instance, it can be included as a comprehensive environment for process design including dynamic operability. In this situation, the optimal operating conditions can be calculated by static optimization and the dynamic behavior can be synthesized afterwards to mitigate the problems of right half plane (RHP) zeros, dynamic coupling, disturbance effects, variability of product quality, etc. In the case of more complex models, it can also be associated with bifurcation analysis tools to provide valuable information for design.

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