8th International IFAC Symposium on
Dynamics and Control of Process Systems
Preprints Vol.2, June 6-8, 2007, Cancún, Mexico

A SIMPLE WAY TO GENERATE DYNAMIC MODELS FROM STATIC SIMULATIONS

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Abstract: The dynamic simulation of processes is much less used in practice for design and analysis than static simulation mainly due to the difficulty and the cost of obtaining a dynamic model. This paper is concerned with the possibilities of generating such representations on the basis of steady-state models, which are easier to develop and therefore more commonly encountered in the engineering practice. The analysis, focused on process control purposes, is based on a generic framework, and the extra work needed to generate a dynamic model from a static one is discussed. A simple computational example is given to illustrate the presented ideas.

Keywords: Dynamic Models; Static Simulation; Steady-State Models; Shortcut Models; Design and Control.

1. INTRODUCTION

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, with applications ranging from operator training to dynamic optimization, the cost of developing such a 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.

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 way of making use of this model for the construction of consistent dynamic extension would be very beneficial. As an example, in some commercial programs the solutions of a stationary model and the corresponding dynamic model at steady-state do not match. 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 with time responses), which are then used for tuning controller parameters. It would be therefore very valuable to have some methodology permitting to bypass the dynamic modeling step and to obtain the corresponding linearized dynamic models directly from the steady-state simulator.

The integration of design and control received much attention in the past years. Methods that allow for the study of input-output controllability issues – that is, poles and zeros of the linearized models, RGA, RPN, etc. (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. Further, controllability issues could be considered together with the design task, leading for example for the optimal holdup in each equipment, with respect both to the control and the profit of the unit.

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 paper is on control and dynamic optimization, we consider solely lumped systems. In the formulation below, it will be assumed for simplicity that the control volumes are well mixed, and that the processes operate isothermally, although proper modifications in the formulation can account for non-isothermal conditions.

This paper is organized as follows: **Section 2** applies the considerations above to systems containing just one species and several control volumes, that is, processes represented by a set of total mass balances. **Section 3** describes how a dynamic model can be determined directly on the basis of the steady-state model, and also what kind of additional information is necessary to perform this, as well as some applications. **Section 4** exploits the somewhat reversal situation of **Section 2**, that is, the case of one single compartment and several species, particularly for systems with chemical reaction. **Section 5** shows an example of the first case cited above. Conclusions are drawn in **Section 6**.

2. SINGLE-SPECIES, HOMOGENEOUS SYSTEMS

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

$$\dot{\mathbf{m}} = k\left(\mathbf{\Phi}_{\text{in}} - \mathbf{\Phi}_{\text{out}}\right) \tag{1}$$

where $\mathbf{m} = [m_1 \;\; m_2 \;\; \ldots \; m_n \,]^T$ is the vector of mass holdups, $\mathbf{\Phi}_{in}$ and $\mathbf{\Phi}_{out}$ are respectively the vector mass flows into and from each compartment, and k is a common factor between $\mathbf{\Phi}_{in}$ and $\mathbf{\Phi}_{out}$ (the reason for letting it explicit will become clear later). It is also assumed for convenience that a single phase is present in the system. This set of ordinary differential equations (ODE's), with proper initial conditions, describes the time evolution of the holdups as a function of the inflows/outflows.

A very common situation is when one is not interested in the mass holdups directly, but in some related quantities given in the vector $\mathbf{q}$ (as for example, liquid levels, gas pressure and so on), which will be called here the *state variables of the problem*. These are related to the mass holdups by means of a relation of the form $\mathbf{m} = \mathbf{\Pi}(\mathbf{q})$, which is assumed to be invertible, at least locally.
In this case, the mass balances can be expressed in terms of the new state variables as

$$\dot{\mathbf{q}} = k\left[\frac{\partial \mathbf{\Pi}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1}\left(\mathbf{\Phi}_{\text{in}} - \mathbf{\Phi}_{\text{out}}\right). \tag{2}$$

The invertibility of the Jacobian matrix above (also called "mass matrix") is guaranteed by the continuous differentiability of $\mathbf{\Pi}$. The flows among the compartments will usually depend on the state variables themselves, and therefore it is possible to write (the symbol "~" expresses formally the dependency of the flows on $\mathbf{q}$):

$$\dot{\mathbf{q}} = k\left[\frac{\partial \mathbf{\Pi}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1}\left(\tilde{\mathbf{\Phi}}_{\text{in}}(\mathbf{q}) - \tilde{\mathbf{\Phi}}_{\text{out}}(\mathbf{q})\right). \tag{3}$$

Moreover, especially for control applications, it is customary to distinguish *manipulated variables* $\mathbf{u}$, which are external to the system and, except in the case of feedback loops, independent of the states:

$$\dot{\mathbf{q}} = k\left[\frac{\partial \mathbf{\Pi}(\mathbf{q})}{\partial \mathbf{q}}\right]^{-1}\left(\hat{\Phi}_{\text{in}}(\mathbf{q},\mathbf{u}) - \hat{\Phi}_{\text{out}}(\mathbf{q},\mathbf{u})\right) \tag{4}$$

where " $\wedge$ " denotes the dependency on $\mathbf{u}$.

2.1 Stationary Models

A static model is the stationary solution of (4), that is, a set of algebraic equations of the form:

$$\hat{\Phi}_{\text{in}}(\mathbf{q},\mathbf{u}) - \hat{\Phi}_{\text{out}}(\mathbf{q},\mathbf{u}) = \mathbf{0}\,. \tag{5}$$

The solutions of this equation are obviously insensitive to any multiplicative factor as k or as the Jacobian matrix in (4). Moreover, as long as there are N independent equations in (5), for a given vector $\mathbf{u}_0$ it is possible to solve the model equations for the steady-state $\mathbf{q}_0$, at least locally. A model of the form (5) in which $\mathbf{q}$ cannot be isolated is said here an *implicit steady-state model*. An *explicit steady-state model* will be considered to be a relationship of the form:

$$\mathbf{q} = \mathbf{\Omega}(\mathbf{u})\,. \tag{6}$$

Eq. (6) above may be an analytical solution of (5), what is not possible in general, or may represent any numerical procedure or black-box model of the steady-state solution, from which it is not possible to recover Eq. (5) entirely.
With this regard, it is possible to admit that the implicit model is just an approximation of the correct solution (as, in fact, all steady-state models are).

3. FROM STATIONARY MODELS TO DYNAMIC ONES

In many cases, it is interesting to develop dynamic models from existing stationary models, as discussed in Section 1. In view of this, two situations can be devised: implicit and explicit steady-state models.

3.1 Implicit steady-state models

Observing (1), it can be realized that the implicit steady-state model (5) corresponds to the right-hand side of the state equation written in terms of $\mathbf{m}$, up to the constant k. Thus, if this model is available, it is possible to generate a dynamic model on its basis, in the following form:

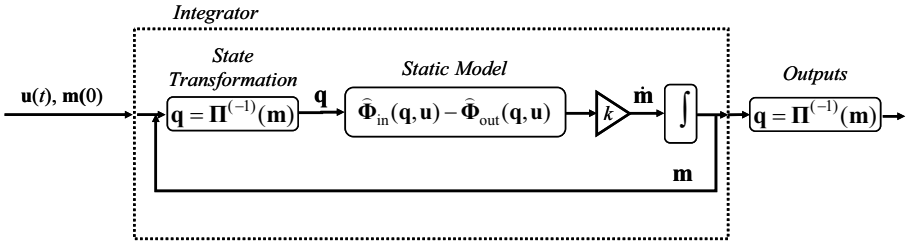

Fig. 1. Schematic representation of the proposed dynamic model

$$\dot{\mathbf{m}} = k\left(\hat{\boldsymbol{\Phi}}_{\text{in}}\left(\boldsymbol{\Pi}^{(-1)}(\mathbf{m}),\mathbf{u}\right) - \hat{\boldsymbol{\Phi}}_{\text{out}}\left(\boldsymbol{\Pi}^{(-1)}(\mathbf{m}),\mathbf{u}\right)\right) \tag{7}$$

with output equation

$$\mathbf{q} = \boldsymbol{\Pi}^{(-1)}(\mathbf{m}) \tag{8}$$

where " $^{(-1)}$ " denotes function inverse. The need for representing $\mathbf{q}$ by $\boldsymbol{\Pi}^{(-1)}(\mathbf{m})$ in (7) comes from the fact that the associated initial value problem will be defined in terms of $\mathbf{m}$ and not in the state variables of the problem ($\mathbf{q}$). Analyzing (7), it is possible to verify that the following extra work will be necessary in order to construct the dynamic model on the basis of (5):

- to obtain the factor k, which will represent any common terms between $\boldsymbol{\Phi}_{in}$ and $\boldsymbol{\Phi}_{out}$. It must be determined from phenomenological considerations;
- to obtain the expression relating the mass holdups of the compartments and the state variables of interest.

These two steps can be understood as an additional modeling effort, necessary to generate the correct holdup terms in the dynamic mass balance. A schematic representation of this model can be seen in Fig. 1.

3.2 Explicit steady-state models

In the case of the explicit steady-state models (6), the work of obtaining a dynamic representation equivalent to (4) is much more difficult because of the probable "loss of structure" implied by the analytical solution of (5), what is necessarily the case for numerical/approximated models. Apart from the few cases when it is possible to recover completely the steady-state equation, an additional step will be required for determining its structure.

In the present work, only the following simple situation will be analyzed: the case of N sub-systems (compartments) in series, with no interconnections excepting between the i-th and the $(i+1)$-th elements, $i = 1,\ldots, N-1$. In also necessary to admit that the (scalar) input u is the mass flow into the first compartment; if this is not the case, it is necessary to find first the relationship $u = g(v)$ between u and the actual input v. Admitting the elements of $\boldsymbol{\Omega}$ in (6) are invertible functions, one can write

$$u = \boldsymbol{\Omega}^{(-1)}(\mathbf{q}) \tag{9}$$

where the inverse can be taken element-wise (this is possible because there is just one global mass balance per compartment). In this case, due to the structure of the system, it is possible to write

$$\begin{aligned} u - \boldsymbol{\Omega}_1{}^{(-1)}(q_1) &= 0 \\ u - \boldsymbol{\Omega}_2{}^{(-1)}(q_2) &= 0 \\ &\vdots \\ u - \boldsymbol{\Omega}_N{}^{(-1)}(q_N) &= 0 \end{aligned} \tag{10}$$

and therefore the following model can be derived, which is in the form of (5):

$$\begin{aligned} u - \boldsymbol{\Omega}_1{}^{(-1)}(q_1) &= 0 \\ \boldsymbol{\Omega}_1{}^{(-1)}(q_1) - \boldsymbol{\Omega}_2{}^{(-1)}(q_2) &= 0 \\ &\vdots \\ \boldsymbol{\Omega}_{N-1}{}^{(-1)}(q_{N-1}) - \boldsymbol{\Omega}_N{}^{(-1)}(q_N) &= 0 \end{aligned} \quad . \tag{11}$$

Besides of an attempt to "recover" (5) from an explicit steady-state model, (11) can be used as a basis for the gray-box identification of a block-oriented dynamic model, as in Pearson and Pottmann (2000), or as discussed in Bolognese Fernandes (2006) and Bolognese Fernandes and Engell (2005).

3.3 Other Application: Taylor 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 system (4), which is of the form:

$$\Delta\dot{\overline{\mathbf{q}}} = \mathbf{A}\cdot\Delta\overline{\mathbf{q}} + \mathbf{B}\cdot\Delta\mathbf{u} \tag{12}$$

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:

$$\begin{aligned} \mathbf{A} = k\frac{\partial}{\partial\mathbf{q}}\left(\left[\frac{\partial\boldsymbol{\Pi}(\mathbf{q})}{\partial\mathbf{q}}\right]^{-1}\right)\left(\hat{\boldsymbol{\Phi}}_{\text{in}}(\mathbf{q},\mathbf{u}) - \hat{\boldsymbol{\Phi}}_{\text{out}}(\mathbf{q},\mathbf{u})\right) + \\ k\left[\frac{\partial\boldsymbol{\Pi}(\mathbf{q})}{\partial\mathbf{q}}\right]^{-1}\left(\frac{\partial\hat{\boldsymbol{\Phi}}_{\text{in}}(\mathbf{q},\mathbf{u})}{\partial\mathbf{q}} - \frac{\partial\hat{\boldsymbol{\Phi}}_{\text{out}}(\mathbf{q},\mathbf{u})}{\partial\mathbf{q}}\right) \end{aligned} \quad . \tag{13}$$

$$\mathbf{B} = k\left[\frac{\partial\boldsymbol{\Pi}(\mathbf{q})}{\partial\mathbf{q}}\right]^{-1}\frac{\partial}{\partial\mathbf{u}}\left(\hat{\boldsymbol{\Phi}}_{\text{in}}(\mathbf{q},\mathbf{u}) - \hat{\boldsymbol{\Phi}}_{\text{out}}(\mathbf{q},\mathbf{u})\right) \tag{14}$$

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 (5) with respect to **q** (all evaluated at the steady-state), since the first term in (13) vanishes for any stationary solution of (4), by virtue of (5).

Moreover, given that the equilibrium points can be parameterized by **u** (which is, at least in principle, of smaller dimension than **q**), it is possible to obtain interpolated versions of $\mathbf{A} = \mathbf{A}(\mathbf{u})$, thus "compacting" the linear representations of the system (Bolognese Fernandes, 2006).

Another possibility with this respect is to consider these parameterized models to formulate control-related 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, etc…) that can be parameterized in terms of the equilibrium points.

4. MULTI-SPECIES, HOMOGENEOUS 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 (Elnashaie and Garhyan, 2003):

$$\dot{\mathbf{n}} = \boldsymbol{\Theta}_{in} - \boldsymbol{\Theta}_{out} + \boldsymbol{\nu} \tag{15}$$

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 flows 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 **c** a more natural state variable, and since $\mathbf{n} = \mathbf{c} \cdot V$, the mole balance (15) becomes:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{c} \cdot V\right) &= V \cdot \dot{\mathbf{c}} + \mathbf{c} \cdot \dot{V} = \\ \boldsymbol{\Theta}_{in} - \boldsymbol{\Theta}_{out} &+ \hat{\mathbf{v}}(\mathbf{c}) \cdot V = \\ \mathbf{c}_{in} \cdot \Lambda_{\mathrm{in}} - \mathbf{c} \cdot \Lambda_{\mathrm{out}} &+ \hat{\mathbf{v}}(\mathbf{c}) \cdot V = 0 \end{aligned} \tag{16}$$

where V is the volume of the reacting mixture and 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 (1), that is:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left(\rho(\mathbf{c}) \cdot V\right) &= \Phi_{\mathrm{in}} - \Phi_{\mathrm{out}} \\ &= \rho(\mathbf{c}_{in}) \cdot \Lambda_{\mathrm{in}} - \rho(\mathbf{c}) \cdot \Lambda_{\mathrm{out}} \end{aligned} \tag{17}$$

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

At steady-state, it is thus possible to write

$$\begin{aligned} &\mathbf{c}_{in} \cdot \Lambda_{\mathrm{in}} - \mathbf{c} \cdot \Lambda_{\mathrm{out}} + \hat{\mathbf{v}}(\mathbf{c}) \cdot V = \\ &\Lambda_{\mathrm{in}} \cdot \left(\mathbf{c}_{in} - \frac{\rho(\mathbf{c}_{in})}{\rho(\mathbf{c})} \mathbf{c} \right) + \hat{\mathbf{v}}(\mathbf{c}) \cdot V = 0 \end{aligned} . \tag{18}$$

Implicit steady-state model. In this case, a model in either forms in (18) can be used to construct a dynamic model by means of the knowledge of the dynamic variations of Λ_{in} and Λ_{out}. The analysis can be coupled here with that in the **Section 3** in order to provide such a relationship (that is, the overall mass balance).

Explicit steady-state model. For the construction of a dynamic model on the basis of an explicit steady-state model $\mathbf{c} = \boldsymbol{\Omega}(\mathbf{u})$, it will be assumed that **u** is the entire vector of feed concentrations ($\mathbf{c}_{in}$), individual molar flow rates ($\Lambda_{in} \cdot \mathbf{c}_{in}$) or any other multiple of them by an scalar factor (the reason for this will become clear). Evidently, in the case of variable mixture volume and/or variable overall feed flow rate, it is required that the steady-state model is of the form $\mathbf{c} = \boldsymbol{\Omega}(\mathbf{u}, \Lambda_{in}/V)$, thus accounting for varying residence time.

In the case that $\mathbf{u} \equiv \mathbf{c}_{in}$, at a given stationary point ($\mathbf{c}_{in,s}$, $\mathbf{c}_s$) we have for the rate term in (18):

$$\begin{aligned} \hat{\mathbf{v}}(\mathbf{c}_s) = &-\frac{\Lambda_{\mathrm{in}}}{V} \cdot \left(\mathbf{c}_{in,s} - \mathbf{c}_s\right) = \\ &-\frac{\Lambda_{\mathrm{in}}}{V} \cdot \left(\boldsymbol{\Omega}^{(-1)}(\mathbf{c}_s) - \mathbf{c}_s\right) \end{aligned} \tag{19}$$

where it was assumed for simplicity that $\rho(\mathbf{c}_{in}) = \rho(\mathbf{c})$. Consequently, at any point ($\mathbf{c}_{in}$, **c**), not necessarily stationary, it is possible to substitute (19) in (16), thus giving:

$$\dot{\mathbf{c}} = \frac{\Lambda_{\mathrm{in}}}{V} \cdot \left(\mathbf{c}_{in} - \boldsymbol{\Omega}^{(-1)}(\mathbf{c})\right) \tag{20}$$

what constitutes a dynamic model of the form (15). Constant mixture volume was assumed for simplicity in the expression above. It is important to notice that, under the previous assumptions, (20) represents no approximation, but an exact relationship. This is due to the fact that **Ω** has (at least locally) a "full" inverse, because the dimensions of its input/output arguments are the same. Geometrically speaking, this means that the projection of any point ($\mathbf{c}_{in}$, **c**) on the phase plane (state-space) will be contained by the projection of the space of equilibrium points itself on the same plane. In other words, for any point ($\mathbf{c}_{in}$, $\mathbf{c}_s$)

it will be possible to find a value of $\mathbf{c}_{in,s}$ such that ($\mathbf{c}_{in,s}$, $\mathbf{c}_s$) is an equilibrium point.

Obviously, it is also possible that this inverse does not exist locally, although this must occur for a countable set of points. The numerical problem of finding the correct solution of the inversion problem in face of output multiplicities will not be considered here.

5. NUMERICAL EXAMPLE: THREE TANK SYSTEM

In this section, it will be shown how a dynamic model of the level system shown schematically in Fig. 2 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 h_i in the tanks [cm], $i = 1, 2, 3$. A stationary model of the system is given by:

$$h_i = \left(F_0 / c_{v,i}\right)^2, \quad i = 1, 2, 3 \tag{21}$$

where $c_{v,i}$ is the valve coefficient.

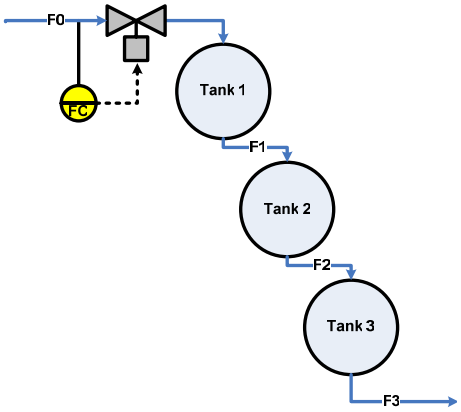

Fig. 2. Diagram of the spherical tank system

The system exhibits nonlinear dynamic features, as displayed in Fig. 3; this is evidenced by the differences of the step responses at the three equilibrium points corresponding to low, medium and high levels in the third thank. These differences of the behaviour are very useful to test the proposed modelling approach.

Implicit steady-state model. Since the system is in compartmental, the analysis in **Section 3.2** can be applied here, thus giving

$$\begin{aligned} F_0 - c_{v,1}\sqrt{h_1} &= 0 \\ c_{v,1}\sqrt{h_1} - c_{v,2}\sqrt{h_2} &= 0 \\ c_{v,2}\sqrt{h_2} - c_{v,3}\sqrt{h_3} &= 0 \end{aligned} \tag{22}$$

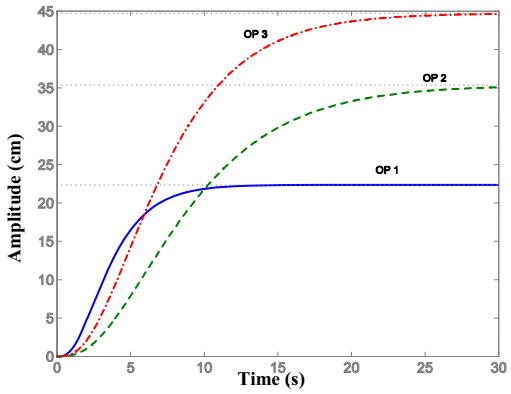

Fig. 3. Step responses of the spherical tank system at three typical operating points

which is in this case exactly the implicit stationary model and therefore in the form of (5).

Dynamic shortcut model. In order to generate a dynamic model on the basis of (22), as described in **Section 3.1**, it is necessary to represent the dependence $\mathbf{m} = \mathbf{\Pi}(\mathbf{h})$ of the holdup in each compartment with the respective level. Since the tanks are spherical, this relationship is given by

$$m_i = \rho \cdot \frac{\pi}{3} \cdot h_i^2 \cdot \left(\frac{3}{2} D_i - h_i\right), \quad i = 1, 2, 3 \tag{23}$$

where ρ was considered constant for convenience. The inverse $\mathbf{\Pi}^{(-1)}$ is the root of a third order polynomial in h_i and has therefore a quite complex form. The extra factor k (recall Eq. (7)) can be seen in this case to be ρ. A model of the form (7) was then constructed in Matlab for the dynamic simulation of this system, resulting in the following equations:

$$\begin{aligned} & m_i - \rho \frac{\pi}{3} h_i^2 \left(\frac{3}{2} D_i - h_i\right) = 0, \quad i = 1, 2, 3 \\ & \dot{m}_1 = \rho\left(F_0 - c_{v,1}\sqrt{h_1}\right) \\ & \dot{m}_j = \rho\left(c_{v,j-1}\sqrt{h_{j-1}} - c_{v,j}\sqrt{h_j}\right), \quad i = 2, 3 \end{aligned} \tag{24}$$

along with output equations as in (23). The algebraic equations above are decoupled from the state equations, in the sense that they can be solved separately for the h_i, and thus the system is not a "true" DAE representation. Observe that the dynamic model (24) is in the form of Fig. 1 and was obtained solely on the basis of (21), which can be in principle a heuristic steady-state model or a "black-box" function, as a compiled routine, for example.

The model (24) was compared with the one obtained by the "traditional", or direct, approach, that is, by directly writing down the dynamic balances:

$$\begin{aligned} \dot{h}_1 &= \frac{F_0 - c_{v,1} \cdot \sqrt{h_1}}{\pi \cdot h_1 \cdot (D_1 - h_1)} \\ \dot{h}_i &= \frac{c_{v,i-1} \cdot \sqrt{h_{i-1}} - c_{v,i} \cdot \sqrt{h_i}}{\pi \cdot h_i \cdot (D_i - h_i)}, \quad i = 2, 3 \end{aligned} \tag{25}$$

The simulations of both models with respect to a given input sequence are depicted in **Fig. 4**. The values of the parameters are given in the Appendix. As it can be expected, both responses are identical, since the models are totally equivalent.

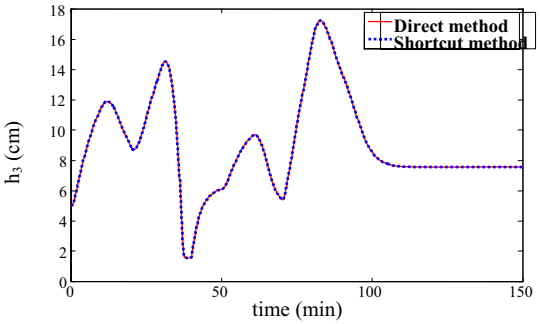

Fig. 4. Dynamic simulation of the three tank system

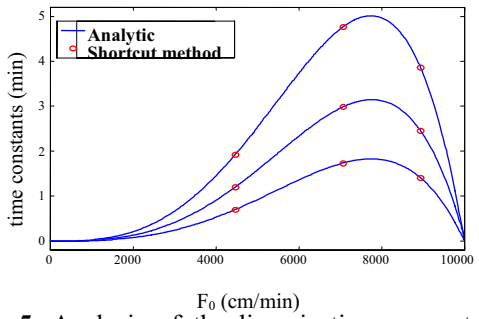

Fig. 5. Analysis of the linearization parameters in terms of the operating points for the three tank system

Linearization analysis. Another interesting application is to employ sensitivity studies of the steady-state model, coupled with the information given by (23), in order to determine the Taylor linearizations of the system, as described in **Section 3.3**. In order to illustrate this, the time constants of three linear models, obtained by this shortcut method at the equilibrium points determined by the feed flow rates of 4470, 7070 and 8940 cm^3/min, are compared with the values determined analytically, as shown in Fig. **5**. Again, since the shortcut method represents no approximation, the results are identical. A numerical procedure (Matlab function `NUMJAC`) was employed in order to generate the sensitivities of the steady-state mass balances with respect to the state variables of the problem at the three operating points.

6. CONCLUSIONS

This paper showed some possibilities of exploiting steady-state information in order to construct dynamic models, as well as the necessary extra information to produce them. The analysis was restricted to lumped, isothermal systems, although, at least in the last situation, extensions seem to be straightforward.

The 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.

APPENDIX

Parameter values used in the example of the three tanks:
$\rho = 1000$ kg/m^3, $D_1 = 35$ cm, $D_2 = 20$ cm, $D_3 = 25$ cm, $c_{v,1} = 0{,}0169$ $m^{2.5}$/min, $c_{v,2} = 0{,}0183$ $m^{2.5}$/min, $c_{v,3} = 0{,}02$ $m^{2.5}$/min.

AKNOWLEDGEMENTS

The authors thank FINEP and PETROBRAS for the financial support.

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