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EFFECT OF STEADY STATE ASSUMPTION ON THE STRUCTURAL SOLVABILITY OF DYNAMIC PROCESS MODELS

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The variable structure of dynamic process models is represented by a directed graph termed the representation graph for the purpose of solvability analysis in this paper. Structural solvability analysis, the determination of the structural differential index and the structural decomposition of the DAE model set can be performed using the representation graph.
It is shown that the effect of steady state assumption for a state variable x can be handled on the representation graph by modifying the assignment of the derivative variable vertex x'. The method enables us to select a suitable modification of the original specification such that the structural solvability and the differential index of index 1 process models remains unchanged.
In the case of index 2 models, a steady state assumption may decrease the differential index of the modified model to 1 if the derivative variable is on the underspecified subgraph. The notions and methods are illustrated on simple process examples.

Keywords: process models, DAE models, differential index, solvability, structural analysis, steady state assumption

Introduction

Lumped process models are in the form of differential-algebraic equations which are sometimes difficult to solve numerically due to index and stiffness problems. Therefore the solvability analysis of differential-algebraic equations (DAE) process models are of primary importance for dynamic simulation.

It is an important related question how high index process models arise. The effect of some decisions taken during the modelling process on the structural solvability has already been investigated in detail [8]. It is known that the change in the specification may transform an index 1 model to a higher index one [4]. It is also known that algebraic transformations, that is transformations which only change the algebraic form of a DAE model may change its structural solvability properties, namely its decomposition in a rather drastic way [6], but they do not change the differential index of the model.

Various methods and techniques have been proposed for structural solvability analysis based on both algebraic (see e.g. [11], [2]) and graphical combinatorial ([9], [12], [10]) techniques. Marquardt *et al.* defined a structural approach to the characterization of DAEs which is derived from symbolical algorithm [11]. In addition to this, two systematically different structural approaches were applied to support the development of low index models.

It is intuitively clear, that modelling assumptions may drastically affect the structural solvability properties of a process model. Therefore it is of primary importance to analyze the effect of widely used model specification assumptions, for example the steady state assumption on the differential index. In order to enlighten the importance and significance of analyzing the solvability properties of process models and the effect of modelling thereon we should recall that modelling is one of the key and most labour-consuming activity in process system engineering serving as a basis for process flowsheeting, process control, fault detection and diagnosis. Modelling assumptions can be seen as artifacts of process modelling being a sequential-iterative procedure with the assumptions coding the decisions of the modeller. In the case of problems with solving the model one is interested in finding the decisions leading to it.

Static and dynamic flowsheeting packages nowadays are almost all equipped with "post mortem" solvability analysis tools but these cannot give advice on how to repair a model with solvability problems. Therefore there is a growing demand from the users of such packages to have an intelligent front-end advisor to help them. The current paper can be regarded as one of the first steps to achieve this ambitious goal.

The graph theoretical method proposed by Murota [9] serves as a basis of the analysis, which can effectively be used for large systems with several hundred variables. This solvability analysis of the model equations gives information on the computation order and on the size of nonlinear sub-sets fo equations to be solved iteratively. Decompositions of the original DAE model are used for detailed solvability analysis.

In our earlier work [6] we used these graph-theoretical methods for index analysis of DAE process models and we developed index reduction techniques for high index models based thereon. The graph representation of DAE process models offers computationally cheap methods for analysing the differential index and structural solvability decompositions which can effectively be used for large systems.

In this paper our aim is to investigate how a steady state assumption for a state variable can be handled on the representation graph and what is the effect of this assumption on the solvability properties of the model in general and on the differential index, in particular.

The paper is organised as follows. We start with basic notion on structural solvability analysis and on the graph representation of DAE process models in the next section. Thereafter the effect of steady state assumption on the differential index is discussed both for index 1 and higher index models. Finally conclusions are drawn.

Basic Notions

The basic notions on structural solvability are described here for both algebraic and DAE models. Related questions, such as the representation of DAE models and the handling of model specifications are also discussed.

From the viewpoint of the solvability, the most important characteristic feature of process models is the differential index which determines the difficulty of their solution. Therefore the basic notions on differential index of DAE models are also discussed in this section.

The structural solvability of a DAE model can be investigated on the so-called representation graph [9].

Structural solvability

As a first step, we consider a *system of linear or non-linear algebraic equations in its so-called standard form* [9]:

$$y_i = f_i(x,u), \quad i = 1,\dots,M \tag{1}$$

$$u_k = g_k(x,u), \quad k = 1,\dots,K \tag{2}$$

where x_j, ($j = 1,\dots, N$) and u_k, ($k = 1,\dots, K$) are unknown, y_i, ($i = 1,\dots, M$) are known parameters, f_i, ($i = 1,\dots, M$) and g_k, ($k = 1,\dots, K$) are assumed to be sufficiently smooth real-valued functions. We assume that the partial derivatives of functions f_i and g_k are elements of a field $\mathcal{F}$ that is an extension of the rational number field $\mathcal{Q}$. The system of equations above is *structurally solvable*, if the Jacobian matrix $J(x, u)$ as a matrix over $\mathcal{F}$, is non-singular, where

$$J(x,u) = \begin{bmatrix} J(f,x) & J(f,u) \\ J(g,x) & J(g,u) - I_k \end{bmatrix} \tag{3}$$

$$J(f,x) = \left[\frac{\partial f_i}{\partial x_j}\right], \quad J(f,u) = \left[\frac{\partial f_i}{\partial u_l}\right] \tag{4}$$

$$J(g,x) = \left[\frac{\partial g_k}{\partial x_j}\right], \quad J(g,u) = \left[\frac{\partial g_k}{\partial u_l}\right] \tag{5}$$

and I_k is the $k \times k$ identity matrix.

It is possible to consider the standard form with no loss of generality in such a way that the variables in left-hand side of equations appear only once [9].

Consider a system of equations in the standard form. We construct a directed graph to represent the structure of the set of equations in the following way. The vertex-set corresponding to unknowns and parameters is partitioned as $X \cup U \cup Y$, where $X = \{x_1,\dots, x_N\}$, $U = \{u_1,\dots, u_K\}$ and $Y = \{y_1,\dots, y_M\}$. The functional dependence corresponding to the equations is expressed by arcs coming into y_i or u_k respectively from those x_j and u_l, which appear on the right-hand side. This graph is called the *representation graph* of the system of equations. It is denoted by $G = (V, A, X, Y)$, where V is the vertex-set, A is the arc-set, X is the entrance and Y is the exit of the graph. The representation graph satisfies the following properties:

1. Each vertex $x \in X$ has no in-coming arcs. (These are initial vertices.)
2. Each vertex $y \in Y$ has no out-going arcs. (These are terminal vertices.)

The representation graph may be regarded as the flow of information in the system as it expresses the existence of functional dependence among variables.

Example 1. Consider the following system of equations:

$$y_1 = f_1(x_1,u_1,u_3) \tag{6}$$

$$y_2 = f_2(u_1,u_3) \tag{7}$$

$$y_3 = f_3(x_2,u_3,u_4) \tag{8}$$

$$u_1 = g_1(x_1,u_2) \tag{9}$$

$$u_2 = g_2(x_1,x_2,u_3) \tag{10}$$

$$u_3 = g_3(u_1) \tag{11}$$

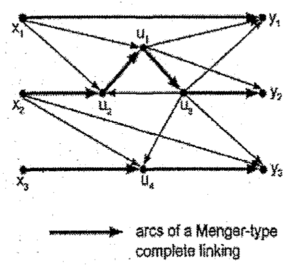


Fig.1 Representation of model in *Example 1*

$$u_4 = g_4(x_2, x_3, u_3) \tag{12}$$

The representation graph of the system above is shown in *Fig.1*.

There is a generality assumption (abbreviated by *GA*) on the functions f_i, $(i = 1,\dots, M)$ and g_k, $(k = 1,\dots, K)$ on which the graphical methods of decomposition are based which is stated as follows:

GA: Let $\mathscr{S}$ be the collection of all partial derivatives of f_i and g_k. The non-vanishing elements of $\mathscr{S}$ are algebraically independent over the rational number field $\mathscr{Q}$.

This assumption means, that the non-vanishing partial derivatives of f_i and g_k are "so general", that they do not satisfy any polynomial relation with integer coefficients.

A *Menger-type linking* [9] from X to Y is a set of pair-wise vertex-disjoint directed paths from a vertex in X to a vertex in Y. The size of a linking is the number of directed paths from X to Y contained in the linking.

In case $|X| = |Y|$, $(M = N)$, a linking of size $|X|$ is called a *complete linking*. The graphical condition of the structural solvability is then the following:

Linkage theorem [9]: *Assume GA is true. A system of equations in the standard form is structurally solvable if and only if there exists on the representation graph a Menger-type complete linking from X to Y.*

In rigorous mathematical sense, the structural solvability and the existence of the Menger-type complete linking are equivalent under the above generality assumption *GA*. In many cases, however, it is difficult to check the validity of this assumption and/or the assumption does not hold at all, therefore we use the property *conditional structural solvability* as follows.

A system of standard form equations is *conditionally structurally solvable* if there exists a Menger-type complete linking from X to Y on the representation graph. Here we do not take into account the generality assumption *GA*. Obviously the conditional structural solvability is a necessary condition of structural solvability.

In further examples we investigate the conditional structural solvability of models.

Example 1 (continued). As shown in *Fig.1* there exists a Menger-type complete linking $\{x_1 \to y_1, x_2 \to u_2 \to u_1 \to u_3 \to y_2, x_3 \to u_4 \to y_3\}$ on the representation graph, so the system described in *Example 1* is structurally solvable under *GA*.

From the viewpoint of structural solvability two types of model decompositions can be defined and constructed using the representation graph. The goal of these decompositions is to obtain the sub-systems of a model and to determine a successful way for solving the model equations.

Representation of dynamic process models

We can adapt the graphical techniques described above to DAE-system, as well [12].

An ordinary differential equation of a DAE system can be described by the following equation:

$$x' = f(x_1,\dots,x_n) \tag{13}$$

Here x denotes an arbitrary variable depending on time, x' denotes the derivative of x with respect to time and $x_1,\dots, x_n$ are those variables which have effect on variable x' in the model.

The variable x of the above differential equation is usually determined using a numerical integration method:

$$x = \int x' dt = \int x' \tag{14}$$

In DAE systems there are two types of variables. *Differential variables* are the variables with their time derivative present in the model. Variables which do not have their time derivative present are called *algebraic variables*. The derivative x' is called *derivative* (velocity) *variable*.

A system of equations including also differential equations, can be represented by a dynamic graph. A dynamic graph is a sequence of static graphs corresponding to each time step of integration. On a dynamic graph there are direct arcs attached from the previous static graph to succeeding static graph corresponding to the method for solving ordinary differential equations.

In case of an explicit method for solving ordinary differential equations the value of a differential variable at a given time is computed using the corresponding differential value and its value at previous time, for example. Therefore if there is an ordinary differential equation $x' = f(x_1,\dots, x_n)$ in the model, we can rewrite it into the following standard form:

$$x = \int x' \tag{15}$$

$$x' = f(x_1,\dots,x_n) \tag{16}$$

The representation graph corresponding to equations (15) and (16) is shown in *Fig.2*. It can be seen that there are vertices on the static graphs referring to the differential variable x, the derivative variable x' and the variables $x_1,\dots, x_n$ occurring in *Eq.(16)*.

Direct arcs attached to static graphs at time step t and t+1 correspond to the applied Euler or other explicit one-step method for solving ordinary differential equations.

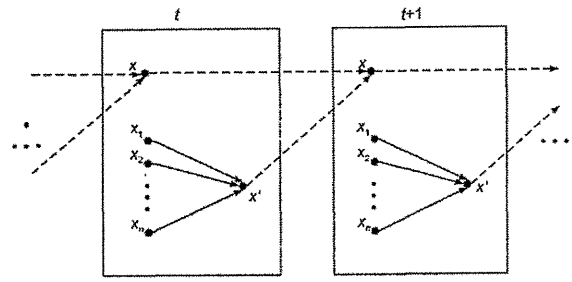


Fig.2 Representation of the structure of an ordinary differential equation by dynamic graph

Standard form and the reduced graph

The form of the representation graph for DAE system models suitable for structural solvability analysis is developed in steps performed sequentially.

The *first step* for investigation of a dynamic process model by the graph theoretical technique *is to rewrite the model into the standard form* (see *Eqs. (1)-(2)* and *(15)-(16)*).

The *second step is the assignment of types to vertices in the representation graph* [5]. The important types of vertices corresponding to the model specification are the following:

- *< S > (set)-type variables*
  These represent variables, which are assigned to the specified given values. These variables require no computation and are present in the specification associated to the process model. The type < S > is usually assigned to initial vertices of the representation graph.
  In case of dynamic representation graph we can assume an explicit Euler method (or another one-step explicit method) for solving the differential equations. Therefore the differential variables will be labeled by type < S > because their initial value can be obtained from the initial conditions then their values can be calculated step by step by numerical integration. In order to distinguish the label < S > assigned to differential variables from the label < S > of other variables with specified given values the label of differential variables is denoted by < S^* >. Labels < S > and < S^* > are treated the same way in the rest of this paper.

- *< G > (given)-type variables*
  A variable assigned to a specific value of a left hand side is a < G >-type variable. Unlike in case of < S >-type variables the values of the right hand side variables will be suitably adjusted so as to preserve the equality of the two sides. The type < G > is usually assigned to terminal vertices of representation graph. A non-terminal vertex assigned to type < G > can be split into two copies one of which being initial and the other which being terminal vertices. The initial vertex is labeled as type < S > and the terminal as type < G >. As a result, vertices of type < G > form a subset of the terminal vertices.

According to the representation graph the value of every variable which has incoming arcs only from vertices labeled by type < S > can be calculated by simple substitution into the corresponding equation. These variables become *secondarily labeled by type < S >*. After this we can calculate the value of all variables which have incoming arcs only from vertices primarily and secondarily labeled by type < S > by simple substitution. These variables will be *tertiarily* labeled by type < S > and this process can be repeated if necessary.

Omitting all vertices labeled primarily, secondarily, etc. by type < S > and all arcs starting from them from the representation graph we obtain the *reduced graph*. The classification of vertices of a reduced graph is as follows:

- all initial vertices form the unknown variable set X,
- all terminal vertices labeled by type < G > constitute the known variable (parameter) set Y,
- all other vertices constitute the unknown variable set U.

Differential algebraic equations and the differential index

The degree of difficulty to solve a DAE-system $F(z(t), z'(t), t) = 0$ can be characterized by the *differential index* of the model. The definition of the differential index [1] is as follows.

The minimum number of times that all or part of a DAE-system $F(z(t), z'(t), t) = 0$ must be differentiated with respect to time in order to determine z' as a continuous function of z and t is the *differential index of the DAE-system.*

Numerical solution of DAEs includes both initialization and integration. To solve DAEs successfully the initial values must be consistent. In case of ODEs the initial values can be chosen independently hence the so called *dynamic degree of freedom* is equal to the number of differential equations. In contrast to this the initial values of DAEs can be constrained by the algebraic equations, so the initialization of DAEs can be cumbersome and the problems related to initialization increase with higher index values. Difficulty of numerical integration of DAEs also increases with higher index values [3].

Dynamic process models can be described by *semi-explicit* DAEs as follows [4]:

$$\dot{z_1} = f(z_1, z_2, t), \quad z_1(t_0) = z_{1_0} \tag{17}$$

$$0 = g(z_1, z_2, t) \tag{18}$$

According to the definition of the differential index a semi-explicit DAE has index one if and only if one differentiation is sufficient to express z'_2 as a continuous function of z_1, z_2 and t. One differentiation is sufficient only if the Jacobian matrix g_{z_2} is non-singular.

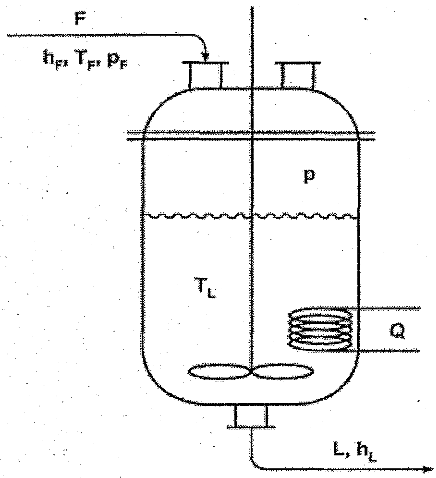


Fig.3 A simple liquid system

Structural non-singularity of gz_2 i.e. the full structural rank of gz_2 results in a model which is *structurally semi-explicit index 1*. The initial values of the differential variables in the semi-explicit index one models may be chosen independently.

If gz_2 is singular then the differential index is greater than 1. Structural singularity of gz_2 is a sufficient condition for differential index being > 1 numerically. In practice most of dynamic process models having differential index > 1 are semi-explicit index 2 models, but there are models having arbitrarily large differential index [8]. The initial values of the differential variables in the higher index semi-explicit models cannot be chosen independently.

High index models can either be simulated directly by an integrator which tackles high index DAEs or be transformed to semi-explicit index 1 model and then integrated.

Investigation of structural solvability of dynamic process models

In our earlier work [7] a graphical technique is presented which is suitable to compute the structural differential index of lumped dynamic process models. The characteristic features of the representation graph of index 1 and high index semi-explicit DAE-models are also described there.

Based on the structural solvability properties a novel index reduction algorithm has been proposed for both index 2 and higher index models. The developed algorithm can also be used for the investigation of the structural differential index and the structural solvability of these models. These results are illustrated on the following example.

Example 2. Consider a liquid tank system with one inlet stream and one exit stream as is shown in *Fig.3*. Let the vessel be perfectly stirred. Heat is transferred to the liquid using a heater. The flow rate and the enthalpy of inlet stream as well as the flow rate of the outlet stream and the heat transfer rate are functions of time.

The model equations of the above system are the following:

$$M' = -L + F \tag{19}$$

$$U' = -L \cdot h_L + F \cdot h_F + Q \tag{20}$$

$$h_L = f_1(T_L, p) \tag{21}$$

$$h_F = f_2(T_F, p_F) \tag{22}$$

$$U = M \cdot u_L \tag{23}$$

$$u_L = f_3(h_L, p) \tag{24}$$

$$L = f_4(M) \tag{25}$$

Here M denotes the mass, U the internal energy, Q heat transfer rate, F and L inlet and outlet mass flow rate, h_F and h_L specific enthalpy of inlet and outlet flow, u_L specific internal energy, T_F temperature of inlet flow, p_F pressure of inlet flow, T_L temperature in the vessel, p atmospheric pressure, respectively and f_1, f_2 and f_3 are given functions.

The standard form of this model is as follows:

$$M = \int M' \tag{26}$$

$$U = \int U' \tag{27}$$

$$M' = -L + F \tag{28}$$

$$U' = -L \cdot h_L + F \cdot h_F + Q \tag{29}$$

$$h_L = f_1(T_L, p) \tag{30}$$

$$h_F = f_2(T_F, p_F) \tag{31}$$

$$u_L = \frac{U}{M} \tag{32}$$

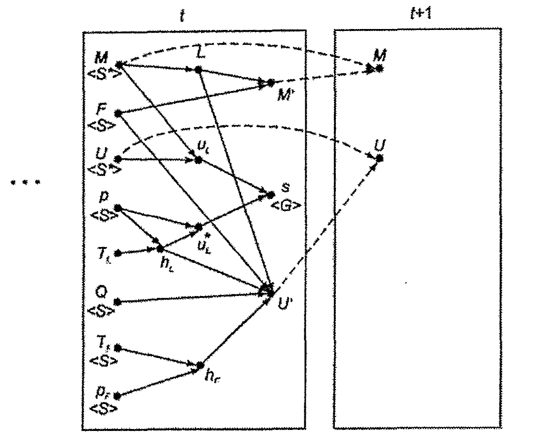
$$u_L^* = f_3(h_L, p) \tag{33}$$

$$s = u_L - u_L^*, \quad s = 0 \tag{34}$$

$$L = f_4(M) \tag{35}$$

Introduction of new variables u_L^*, s and the equation $s = u_L - u_L^*, s = 0$ into the original model guarantees that all variables on the left-hand side of the model are different. In *Eq.(34)* the "satellite" note $s = 0$ refers to the fact that the value of variable s is set to 0, i.e. the variable vertex s is labeled by type $< G >$. The representation graph of the liquid tank system is shown in *Fig.4a*.

We indicate differential variables on the static graph at time step t+1 only, but the structure of this graph is the same as the structure of static graph at time step t.



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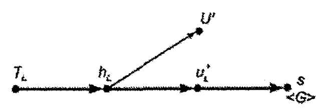

b,

Fig.4 Representation of model with *Specification 1* in *Example 2*; *a,* Representation graph; *b,* Reduced graph

Furthermore, consider the following specification.

Specification 1.

Given: - the properties of the inlet flow F, T_F, p_F and the heat transfer rate Q as functions of time;
- the initial values of mass and internal energy M_0, U_0 and the pressure p are constants;

To be calculated: - the mass, the internal energy and temperature of the liquid in the vessel and the outlet flow rate M, U, T_L, L as functions of time.

It can be shown that the differential index of this semi-explicit DAE system is equal to 1. Dynamic degree of freedom is 2, so initial values of mass M and internal energy U can be chosen independently.

The types of variables assigned corresponding to *Specification 1* are shown in *Fig.4a*. The reduced graph according to *Specification 1* is shown in *Fig.4b*.

Having produced reduced graph, the variable classes related to it can also be given (see the general standard form model (1) - (2)) as follows:

$$X = \{T_L\} \tag{36}$$

$$Y = \{s\} \tag{37}$$

$$U = \{h_L, u_L^*, U'\} \tag{38}$$

and the existence of the Menger-type complete linking can be investigated. It can be seen that there exists a Menger-type complete linking on the reduced graph hence the model is conditionally structurally solvable.

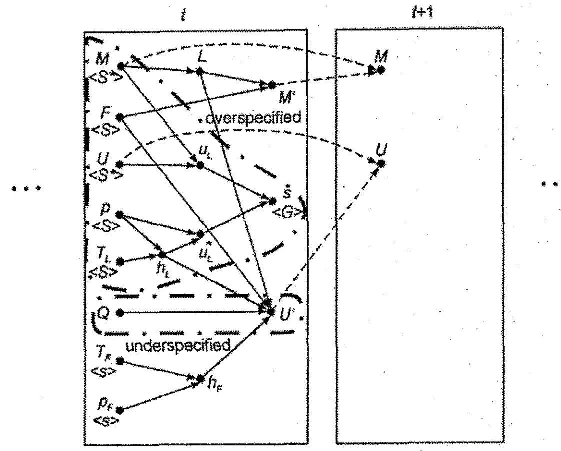

Fig.5 Representation graph of model with *Specification 2* in *Example 2*

Next let us consider the following specification:

Specification 2.

Given: - F, T_F, p_F, T_L as a function of time;
- M_0, U_0, p constants;

To be calculated: - the mass, the internal energy of the liquid in the vessel, the heat transfer rate and the outlet flow rate M, U, Q, L as functions of time.

It is easy to show that the model with *Specification 2* is a semi-explicit index 2 model, because the unknown variable Q is not present in the algebraic equations, so two differentiations are needed to express Q'. The dynamic degree of freedom is 1, so initial values of mass and internal energy can not be chosen independently.

The types of variables which are assigned corresponding to *Specification 2* are shown in *Fig.5*.

Based on the structure of the representation graph on *Fig.5* the following structural solvability properties can be determined.

1. The standard form model is not structurally solvable. (There is no Menger-type complete linking on the graph.)
2. There are an *overspecified part* and an *underspecified part* on the representation graph. The overspecified part indicates the fact that the initial values of the model can not be chosen independently. The underspecified part $Q \to U'$ indicates, that Q can not be calculated from the algebraic equations, so the index of the model is > 1.

The following theorem holds generally [7].

Theorem: Consider a dynamic process model $\mathfrak{M}$ in the standard form described by a semi-explicit DAE system. Assume that the generality assumption *GA* is true. *Then the differential index of* $\mathfrak{M}$ *is equal to 1 if and only if* *there exists a Menger-type complete linking on the reduced graph at any time step t.*

Consequence: Under the assumptions of *Theorem* above the following statement holds. If the differential index of $\mathfrak{M}$ is greater than 1 then there is no Menger-type complete linking on the static graph at any time step *t*.

The properties of a static graph of a dynamic model which has differential index > 1 are as follows.

1. The fact that the initial values of integral variables can not be chosen independently results in an overspecified part on the graph. This situation can be easily shown by assignment of types to vertices corresponding to the model specification. There is an overspecified part on the graph if a vertex labeled by type $< G >$ can also be labeled secondarily or tertiarily or etc. by type $< S >$.
2. Non-singularity of g_{z_2} results in an underspecified part on the graph. In this part those algebraic variables appear which can not be calculated from algebraic equations and those differential variables which we want to calculate from them.

There is a natural method for index reduction suggested by the structure of the representation graph of semi-explicit DAE-systems.

Example 2 (continued). Consider *Example 2* with *Specification 2.* This model has differential index 2. Modify the standard form of the model as follows:

Instead of equation $U = \int U'$ introduce the following equation:

$$U' = U^{t+1} - U^{t} \tag{39}$$

where U^t and U^{t+1} denote the value of internal energy U at time step t and t+1, respectively. This equation corresponds to *numerical derivation* so if we get the derivative U' by numerical derivation we can calculate Q from it.

According to the above transformation of the standard form, let the *modified standard form* of model of *Example 2* be the following:

$$M = \int M' \tag{40}$$

$$M' = -L + F \tag{41}$$

$$U' = -L \cdot h_L + F \cdot h_F + Q \tag{42}$$

$$U'^{*} = U^{t+1} - U^{t} \tag{43}$$

$$s = U' - U'^{*}, \quad s = 0 \tag{44}$$

$$h_L = f_1(T_L, p) \tag{45}$$

$$h_F = f_2(T_F, p_F) \tag{46}$$

$$U = M \cdot u_L \tag{47}$$

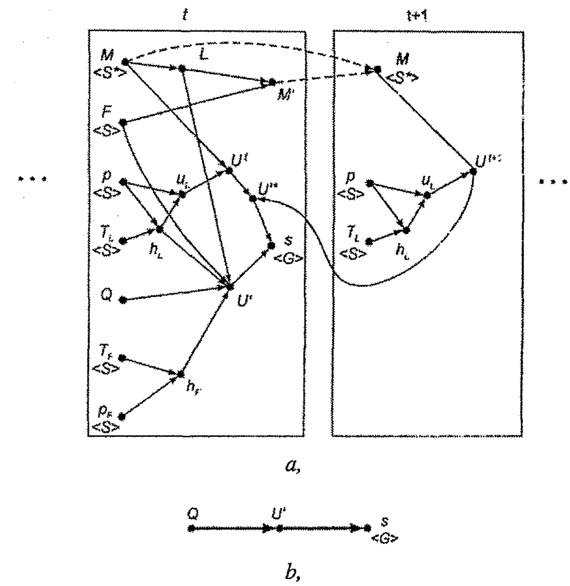

Fig.6 Representation of modified model in *Example 2*; *a,* Representation graph; *b,* Reduced graph

$$u_L = f_3(h_L, p) \tag{48}$$

$$L = f_4(M) \tag{49}$$

During the modification the internal energy U turns from a differential variable into an algebraic variable and U' turns from a derivative variable into an algebraic one. An important consequence of the modification is that there is no integration for variable U in the modified model, so *it is not necessary to give initial value for the variable U.*

The representation graph of the modified model can be seen in *Fig.6a*.

The static graph at time step t+1 shows vertices belonging to variables only, which are necessary to calculate Q in time step t. The reduced graph is shown in *Fig.6b*.

It can be seen that there exists Menger-type complete linking on the reduced graph, so the modified model is conditionally structurally solvable.

Inspired by the above example we generalized the idea of using the "reverse information flow" for computations for a wide class of semi-explicit DAE systems and formulated a general index reduction algorithm [7].

The effect of steady state assumption

Models of complex dynamic systems are often large-sized and complicated. In order to obtain process models of a reasonable size we most often use model simplification. The most frequently applied model simplification assumption originates from the steady state circumstances valid for a state variable. Our aim is to investigate how the effect of steady state assumption can be described on the representation graph of process models and what is the effect of this assumption on the structural solvability, model specification and differential index.

Steady state assumption applied for models with differential index 1

Consider a dynamic process model described by a semi-explicit DAE-system with differential index 1. A state variable of this model can be considered being in steady state if its change in time is approximately equal to 0, compared to the other terms of the differential equation:

$$x' = \frac{dx}{dt} \approx 0 \qquad (50)$$

This fact can be treated on the representation graph in such a simple way, that the assignment of the derivative variable x' becomes type < G >, because the value of x' is equal to zero. The effect of this modification to the structural solvability can be summarized as follows:

Proposition 1: Consider a dynamic process model described by a semi-explicit DAE system in standard form. Let the differential index of this model be 1. Assume that the generality assumption *GA* is true. Assume that the size of Menger-type complete linking on the static graphs of the dynamic representation graph of the model is equal to *k*.

Assume, that the state variable x is in steady state. Let us modify the assignment of the vertex of the derivative variable x' to type $< G >$. Then

1. The static graphs become overspecified at any time step t, hence there are no Menger-type complete linking on them, therefore the model is not structurally solvable.
2. Modify the model specification as follows. Consider that there exists a variable x_j on the static graph which is labelled by $< S >$ or $< S^*$ and there is a directed path from x_j into x' which is vertex-disjoint to paths of a Menger-type complete linking on the original graph. Drop the label $< S >$ or $< S^*$ of variable x_j. After this:

   There is a Menger-type complete linking on static graphs at any time step t, so the model is structurally solvable. The size of the Menger-type complete linking is equal to $k+1$.

Proof: Let G be the static graph of the original dynamic model at time step t and let G' be the modified static graph.

1. There is a Menger-type complete linking on the original static graph G, hence the elements of variable sets X and Y are equal to each other: $|X| = |Y| = k$. During the modification of the assignment of variable x', the number of variables labelled by type $< G >$ increases. Hence G' becomes overspecified, so there is no Menger-type complete linking on it.

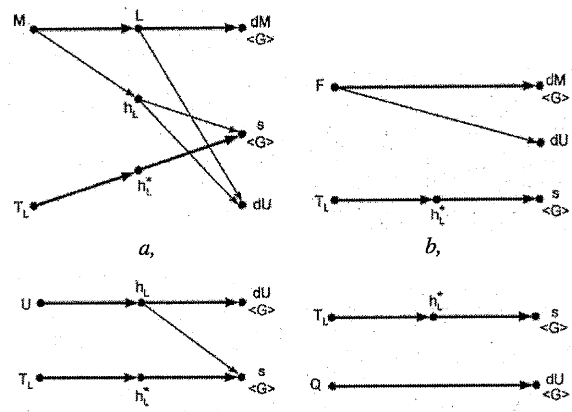

Fig.7 Reduced graph of model in *Example 2* with *Specification 1*; *a,* Assuming steady state for *M* (M_0 is considered to be unknown); *b,* Assuming steady state for *M* (*F* is considered to be unknown); *c,* Assuming steady state for *U* (U_0 is considered to be unknown); *d,* Assuming steady state for *U* (*Q* is considered to be unknown)

2. Changing the model specification the way described above, the following is true on the reduced graph of G': $|X'| = |Y'| = k+1$ and there is a directed path from x_j into vertex x', which gives a Menger-type complete linking on G' with a suitable Menger-type complete linking on the reduced graph of G.

Consequence: Changing the variable assignment (and the model specification) according to Proposition 1 above, *the differential index of the dynamic model does not change.*

Example 2 (continued). Consider *Example 2* with *Specification 1.*

1. Assume, that the mass in the tank is in steady state, that is

   $$M' \approx 0 \qquad (51)$$

   According to the above, this assumption can be treated on the representation graph by modifying the assignment of vertex M' in such a way that it is labelled by type $< G >$. After this, all static graphs become overspecified. According to *Fig.4a* there exist two vertices (*M* and *F*) on the representation graph which are labelled by type $< S >$ or $< S^* >$ and from which a directed path starts into vertex M'. Both of these paths are vertex-disjoint with the Menger-type complete linking of the original reduced graph (see *Fig.4b*). Hence there are two possibilities to modify specification according to Proposition 1. Either the initial value of mass M_0 or the inlet mass flow rate *F* can be unknown, so the original label of one of these vertices can be dropped on the representation graph. With these modifications the new reduced graphs can be seen in *Figs.7a* and *7b*.

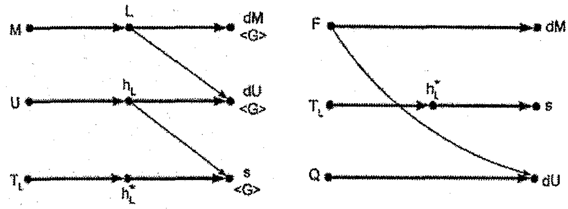

Fig.8 Reduced graph of model in *Example 2* with *Specification 1* assuming steady state for M and U; *a*, M_0 and U_0 are considered to be unknown; *b*, F and Q are considered to be unknown

In both cases there is a Menger-type complete linking on the reduced graph, so the model is conditionally structurally solvable. The size of Menger-type complete linking increases from 1 to 2.

2. Consider that the internal energy of liquid in the tank is in steady state, that is

$$U' \approx 0 \tag{52}$$

Let the value of the derivative variable U' be equal to zero, so it becomes to be labelled by type $< G >$. It can be seen in *Fig.4a* that there are six vertices (M, F, U, T_L, p_F and Q) on the static graph which are labelled by $< S >$ or $< S^* >$ and from which a directed path starts to vertex U'. Dropping the label $< S >$ or $< S^* >$ of any of these vertices is suitable to obtain a conditionally structurally solvable model. *Figs.7c* and *7d* show the reduced graphs of the modified model. In the first case variable U while in the other case variable Q is unknown.

3. Assume, that both the mass and the internal energy of liquid are in steady state in the tank:

$$M' \approx 0 \quad \text{and} \quad U' \approx 0. \tag{53}$$

In this case both vertex M' and vertex U' become labelled by type $< G >$ because of their values are equal to zero. For the appropriate modification of the model specification two vertices must be found on the original representation graph (*Fig.4a*) which are labelled by type $< S >$ or $< S^* >$ and from which two directed paths start into M' and U'. These paths must be vertex-disjoint with the original Menger-type complete linking (see *Fig.4b*). Let M and U or F and Q be the chosen variable pairs. Dropping the original label of these vertices means that these variables are considered to be unknown. Reduced graphs are shown in *Figs.8a* and *8b*.

Assuming steady state for a state variable x, the most usual modification of the specification in the modelling practice is to drop the initial value of variable x from the specification. The above example illustrates that there can be many other modifications of the specification which yield a structurally solvable model. The representation graph is a very suitable tool to find these possible modifications of the original specification.

Steady state assumption for models with differential index 2

Consider a dynamic process model described by a semi-explicit DAE system, which has differential index 2. The representation graph corresponding to the standard form of the model contains an underspecified and an overspecified part. Assume that a state variable x being on the underspecified subgraph is in steady state. Then the following proposition is true.

Proposition 2: Consider a standard form dynamic model described by a semi-explicit DAE-system, which has differential index 2. Assume that the generality assumption *GA* is true for the algebraic part of the model. Consider the dynamic representation graph of the model. Assume that there is only one initial vertex without label $< S >$ on the underspecified part of static graphs. Let x' be a derivative variable also on the underspecified subgraph. Assume that the state variable x is in steady state, so let the value of derivative variable x' be equal to zero. Hence let the label of x' be type $< G >$. Then:

1. Static graphs at any time step t are overspecified, hence there are no Menger-type complete linking on them.
2. Modify the specification of the model as follows: Look for a variable vertex x_k on the overspecified part which has label $< S >$ or $< S^* >$ and drop this label of x_k. Then x_k becomes an unknown variable. The modified model is then structurally solvable.

Proof:

1. It follows from the procedure in Proposition 2 that the overspecified subgraph is unchanged while the underspecification of the originally underspecified part disappears.
2. Variable x' has label $< G >$ therefore there is a directed path from an initial vertex having neither label $< S >$ nor $< S^* >$ into vertex x' on the originally underspecified subgraph. Furthermore, there is a new directed path from x_k into a vertex with label $< G >$ on the originally underspecified subgraph as result of the described modification of specification. These directed paths together with a maximal Menger-type complete linking of the original graph yield a Menger-type complete linking on the modified graph. Hence the modified model is structurally solvable.

Consequence: *The differential index of modified model corresponding to Proposition 2 decreases from 2 to 1.*

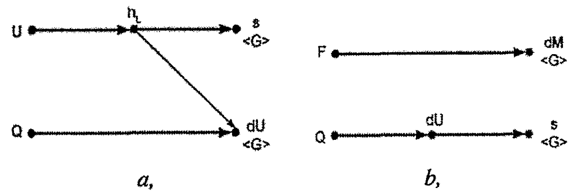

Fig.9 Reduced graph of model in *Example 2* with *Specification 2; a,* Assuming steady state for *U; b,* Assuming steady state for *M*

Example 2 (continued). Consider *Example 2* with *Specification* 2. The differential index of this model is equal to 2. Assume that the internal energy of liquid is in steady state in the tank:

$$U' \approx 0 \tag{54}$$

Then the value of derivative variable U' is equal to zero, so let the label of vertex U' be type $< G >$ on all static graphs. Hence the underspecification of the originally underspecified subgraph disappears. Modify the model specification according to Proposition 2. There are 4 vertices with label $< S >$ or $< S^* >$ (M, U, T_L and p) on the overspecified subgraph (see *Fig.5*). Drop the label $< S^* >$ of vertex U for example, i.e. consider the initial value of internal energy of liquid to be unknown variable in the tank. The reduced graph of modified model can be seen in *Fig.9a*.

There is a Menger-type complete linking on the reduced graph, so the standard form of modified model is conditionally structurally solvable. Hence the differential index of the modified model is equal to 1. The result is the same if we drop the labels of M, T_L or p during the modification of specification. It can be seen, that *the differential index of the standard model decreases from 2 to 1 during the steady state assumption of internal energy of liquid and with the proposed modification of model specification.*

Consider a dynamic process model with differential index 2. Assume that the derivative variable x' does not exists on the underspecified subgraph corresponding to the standard form. Assume that the state variable x is in steady state. Consider the model modified by the index reduction algorithm and its representation graph for this case. Let the value of x' is equal to zero hence the vertex x' becomes type $< G >$. The effect of this modification on the structural solvability is similar to the case of index 1 models as the following example illustrates.

Example 2 (continued). Consider again *Example 2* with *Specification 2.* Assume that the mass of liquid is in steady state in the tank:

$$M' \approx 0 \tag{55}$$

Since the vertex M' does not exist on the underspecified part corresponding to standard form (see *Fig.5*) consider the representation graph belonging to the model modified by the index reduction algorithm (see *Fig.6a*). Let the value of variable M' be equal to zero, hence the vertex M' has label $< G >$ on all static graphs. Look for a vertex with label $< S >$ or $< S^* >$ from which there is a directed path into M'. This directed graph must be vertex-disjoint to the paths of Menger-type complete linking of modified model (see *Fig.6b*). There are two vertices (M and F) which are suitable under the above conditions. Choosing the vertex F and dropping its label $< S >$ the inlet flow rate of liquid is to be considered as an unknown variable. The reduced graph corresponding to the modified model can be seen in *Fig.9b*.

The size of linking increases from 1 to 2. The modified model is conditionally structurally solvable. It can be seen that *the steady state assumption for the mass of liquid in the tank does not change the differential index of the model.*

Conclusion

It is shown in this paper that a steady state assumption for a state variable x of a dynamic process model can be handled on the representation graph by modifying the assignment of the derivative variable vertex x'. The value of x' is equal to zero hence vertex x' becomes type $< G >$.

This modification of the original model results in an overspecified model therefore we must change the model specification to obtain structurally solvable model. After this modification of the specification the differential index of originally index 1 model does not change.

In case of index 2 models two different cases are considered. If the derivative variable vertex x' is on the underspecified subgraph corresponding to the original standard form model, then the standard form of modified model becomes structurally solvable, i.e. the differential index decreases from 2 to 1. If this is not the case, then the effect of a steady state assumption is the same as for the index 1 case.

It was shown that the applied graph theoretical method for structural analysis of DAE process models can be used effectively for investigation of the effect of modelling assumptions.

Further work is directed towards analyzing the effect of other modelling assumptions on the structural solvability properties in general and on the differential index, in particular. Such results may guide the modeller on which assumptions have decreasing effect on the differential index and warn him/her about assumptions which can increase the index.

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