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Index analysis and reduction of systems of quasi-linear partial-differential and algebraic equations

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ABSTRACT

To reliably solve PDAE models in established equation-oriented modeling environments (i) certain mathematical properties are to be fulfilled and (ii) the specified initial- and boundary conditions are to be consistent. For an assessment of both of these aspects an important theoretical framework is the concept of index. In this contribution we propose a new method for a systematic index reduction of quasi-linear PDAE systems. The general idea is to reveal quasi-linear combinations of the differential quantities in the high-index model which are invariant with respect to a specific independent variable. By using these quasi-linear combinations as templates for symbolic manipulations, additional algebraic constraints become explicit. These explicit constraints are then used for index reduction yielding low-index PDAE models. The procedure is demonstrated in the context of a typical modeling work-flow for modeling problems of a tubular reactor, diffusive charge transport in electrolyte mixtures and incompressible fluid flow.

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1. Introduction

Rigorous models for the description of transport phenomena in chemical processes frequently result in systems of partial differential and algebraic equations (PDAE) (Bird et al., 2002; Curtiss and Bird, 1999; Martinson and Barton, 2001). For the numerical treatment of PDAE systems various equation-oriented modeling environments (e.g. Process Systems Enterprise, 1997–2009; Aspentech, 1994–2013) provide suitable methods which are based on the semi-discretization of the PDAE in the spatial coordinates in a method of lines (MOL) approach and the numerical integration of the resulting system of differential-algebraic equations (DAE).

The development of these generic numerical techniques results in an increasing application of detailed distributed models in the form of PDAE systems in simulation, model-based design and control. However, two major challenges can be identified complicating the use of these models: (i) The generic numerical treatment fails easily, if the PDAE system is not characterized by certain mathematical properties. It is generally required that the PDAE system is well-posed in the sense of Hadamard (Vitillaro and Fiscella, 2013; Hadamard, 1902) demanding a consistent specification of initial and boundary conditions. Further, depending on the specific numerical methods applied, additional requirements arise with respect to the structural properties of the PDAE system. (ii) Especially when large and strongly coupled models are concerned, important physical principles are not explicitly depicted in the model structure. Hence, even if a numerical solution is obtained in a straightforward manner, it is difficult to develop a proper relation between the model states and the physical phenomena.

These challenges emphasize the importance of a systematic approach to derive a well-posed distributed simulation model for a given physical system. A typical work-flow used for such a systematic model development is shown in Fig. 1 (Marquardt, 1994). Here, the model developed by established modeling paradigms in step 1 is subject to a theoretical analysis in step 2. The first objective of this analysis is the identification of important mathematical model properties. The second objective is to analyze the model with respect to the physical interpretation of the states in the model. In step 3 the final simulation scenario is specified by formulating appropriate initial and boundary conditions as well as model parameters and input functions. The significance of such a structured modeling approach even for small apparently simple distributed models is illustrated in the following example.

Example 1 *(Isothermal tubular reactor).* An isothermal tubular reactor is considered in which the reactions

$$A + B \overset{r_1}{\rightleftharpoons} C, \tag{1}$$

$$B \overset{r_2}{\rightarrow} D, \tag{2}$$

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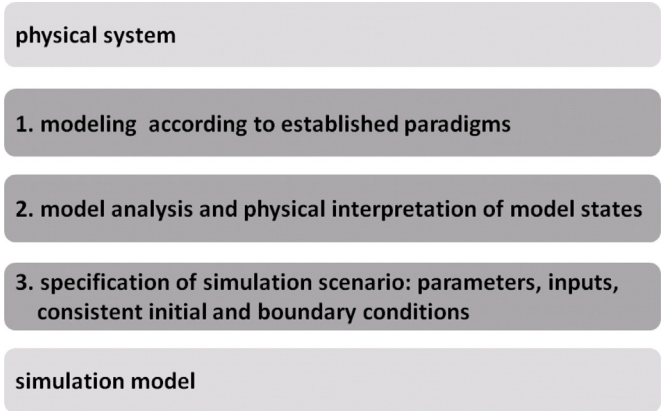

Fig. 1. A general work-flow for the modeling of distributed models.

take place. Assume that the PDAE system

$$\frac{\partial c_k}{\partial t} = -\frac{\partial J_k}{\partial x} - v\frac{\partial c_k}{\partial x} + s_{k,1}r_1 + s_{k,2}r_2, \quad k \in \{A, B, C, D\}, \tag{3}$$

$$J_k = -D^{ax}\frac{\partial c_k}{\partial x}, \quad k \in \{A, B, C, D\}, \tag{4}$$

$$0 = K - \frac{c_A c_B}{c_C}, \tag{5}$$

$$0 = r_2 - k c_B, \tag{6}$$

can describe the system with adequate accuracy if a consistent set of initial and boundary conditions is added. Eq. (3) corresponds to balance equations for the species A, B, C and D in the reaction mixture. The fluxes J_k, accounting for axial dispersion, are introduced by Eq. (4). The mass-action law (5) is introduced to describe the equilibrium reaction (1) by means of the equilibrium constant K. The kinetics of the second reaction (2) are described by the first-order rate law (6) with the reaction rate coefficient k. The stoichiometry of the reactions is captured by the stoichiometric coefficients $\mathbf{s}_1 = [-1, -1, 1, 0]^T$ and $\mathbf{s}_2 = [0, -1, 0, 1]^T$. Further, c_k is the volumetric concentration, v is the velocity of the reaction mixture and D^{ax} is the axial dispersion coefficient. r_1 and r_2 are the net reaction rates.

On first inspection, the model (3)–(6) which consists of 10 scalar equations appears to constitute no particular challenges neither for the physical interpretation of the model states nor for the numerical treatment in established modeling environments. However, a first problem might get apparent when addressing the question which initial and boundary conditions are to specified to complete the problem formulation. The number of differential states in Eqs. (3) and (4) might lead to the assumption that four initial conditions, e.g., one for each concentration, and in total eight boundary conditions can be specified independently. However, as shown in the following such a specification is inconsistent. With a certain amount of experience in modeling dynamic systems this inconsistency might be discovered right away by reasoning that the equilibrium constraint (5) couples three of the four apparently independent concentrations. However, even if this issue is identified right away, no ad hoc solution is available to overcome this problem.

Problems will certainly arise when the numerical treatment of the model (3)–(6) is directly addressed with standard methods. The application of a standard finite-difference scheme to discretize the spatial coordinates in a method of lines approach, e.g. the central finite-difference method (Strikwerda, 2004), implicating the specification of the eight boundary conditions, will yield a singular DAE model which cannot be solved at all. If a well-posed DAE model can be obtained, e.g., by applying a modified discretization scheme, it is very likely that a standard DAE integrator will fail as a consequence of the inconsistent specification of four initial conditions and the structural properties of the model (3)–(6).

In recent works (Martinson and Barton, 2000; Neumann and Pantelides, 2008; Neumann, 2004; Angermann and Rang, 2007) powerful concepts have been developed to assess important mathematical properties of the model and to support the consistent specification of initial and boundary conditions. An important theory in this context is the concept of the differential or perturbation index. Different definitions of these indices are reviewed in detail in Section 2. The essence of the concept of index is to distinguish PDAE systems that are characterized by a weak coupling of the partial-differential and the algebraic part from those where this coupling is more involved. The latter case is commonly denoted as a PDAE characterized by high index behavior.

In general, high index behavior is associated with several problems: (i) From physical considerations it would be expected that all differential quantities with respect to time characterize the storage of extensive quantities and determine the dynamics of the system. However, some of these terms are coupled implicitly and the number of dynamic degrees of freedom is smaller than the apparent number of states occurring as differentials with respect to time. Likewise, not all states appearing in the model formulation as differential quantities with respect to the spatial coordinates show the behavior of evolution variables in space (Martinson and Barton, 2001; Johannink et al., 2011). (ii) Correspondingly, the specification of a consistent set of initial and boundary conditions is subject to "hidden" constraints, which are generally not satisfied by an intuitive approach (Neumann and Pantelides, 2008). (iii) Many of the established numerical methods for the integration of the DAE resulting after the discretization of the spatial coordinates require an index not exceeding one. If applied to high index DAE models, these methods will exhibit order reduction (Hairer et al., 1993), completely fail (Gear and Petzold, 1984), or will yield numerical solutions with an unbounded error (Petzold, 1982). Numerous methods have been recently developed (e.g. Rang and Angermann, 2008; Lang and Verwer, 2001) that are applicable to high index DAEs, which however, are not available in the established modeling environments.

All these critical aspects can be overcome if it is possible to derive equivalent model formulations which are characterized by indices not exceeding one. Such procedures are commonly known as index reduction. However, especially if the considered PDAE systems are large, this is a non-trivial task: The reduction of the index by remodeling (e.g., changing the reference frame or dropping a simplifying assumption) involves knowledge in numerical analysis, profound insight into the underlying physical phenomena and advanced modeling skills. An algorithmic index reduction usually increases the size – e.g., by introducing dummy-derivatives (Mattsson and Soderlind, 1993) – or the complexity – e.g., by repeated differentiation and substitution (Unger et al., 1995) – of the model. Thus, the numerical treatment is more involved and – more importantly – the explicit relation between the model states and the physical phenomena gets easily lost.

In this contribution, we propose a new method for a systematic index reduction of quasi-linear PDAE systems (Zauderer, 2006). We achieve this by generalizing concepts for index reduction of differential-algebraic equations developed by Asbjørnsen and Fjeld (1970), Bachmann et al. (1990) and Moe (1995). The general idea of the reduction method is to reveal quasi-linear combinations of the differential quantities in the high-index model which are invariant with respect to a specific independent variable. By using these quasi-linear combinations as templates for symbolic manipulations applied to the differential equations in the model, additional algebraic constraints become explicit. As these quasi-linear operations preserve the physical information of the original differential

equations, these hidden constraints can be used to substitute differential equations in order to reduce the index. In that manner, the reduction method does not increase the number of equations in the PDAE system. Further, the symbolic manipulations applied to the modeling equations are constructed to eliminate invariant terms and thus are simplifying the model. As the reduction method is based on simple linear algebra concepts and symbolic manipulation, it can easily be implemented in a procedural manner.

The proposed method yields a reformulated PDAE system that is characterized by differential indices of one, which is an important prerequisite for the applicability of many MOL-based numerical methods. Further, since the additional constraints reduce the number of independent differential quantities in the model, the method provides valuable information for the specification of consistent initial and boundary conditions. Moreover, important information is obtained regarding those extensive quantities, which are invariant with respect to a specific independent variable, and hence reveal important physical principals represented in the model. As such, we consider the reduction method as a key component in any work-flow for the development of distributed models.

The remainder of the paper is organized as follows: First, different concepts of index analysis of DAE and PDAE systems are reviewed in Section 2. In this context, different definitions of index are introduced and evaluated as a concept to support the modeling process, the numerical treatment *and* the physical interpretation of PDAE systems. In Section 3, the underlying theory of the index reduction procedure is introduced and illustrated. In Section 4 the role of the reduction method as a major task in any modeling workflow is discussed. Finally, to emphasize its generality, the method is applied in a modeling process to exemplary PDAE systems in Section 5.

2. Index concepts for DAE and PDAE systems

In this section, we briefly introduce the established index concepts for DAE systems and their generalization to PDAE systems. As most of the indices are defined for specific scenarios and require a tailored terminology, the description is restricted to a conceptual level. For a formal description of the concepts, we refer to the original publications.

2.1. Index concepts for DAE systems

The concept of an index has initially been developed for the characterization of DAE systems (Petzold, 1982; Gear and Petzold, 1984). In the most general case, a DAE system is represented in the nonlinear implicit form $\mathbf{F}\left(\mathbf{z},\ \frac{\partial \mathbf{z}}{\partial t},\ \mathbf{u}\right) = \mathbf{0}, \mathbf{z}(t) \in \mathbb{R}^{n_z}, \mathbf{u}(t) \in \mathbb{R}^{n_u}, \mathbf{F}: \mathbb{R}^{n_z} \times \mathbb{R}^{n_z} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}^{n_z}$. Here, $\mathbf{z}(t)$ represents the vector of unknown state variables; $\mathbf{u}(t)$ is the vector of known inputs.

In the mathematical and application-oriented literature, a large number of different indices have been defined. Different definitions are reviewed in detail in Campbell and Marszalek (1999) and Gear (1990). Principally, two index definitions are to be distinguished: the differential index ν_d and the perturbation index ν_p. The perturbation index ν_p introduced by Hairer et al. (1989) represents a quantitative measure of the sensitivity of the solution with respect to the model structure and can be seen as the key quantity characterizing the effort associated with a numerical solution of the DAE system (Unger et al., 1995; Bujakiewicz and van den Bosch, 1994). However, the quantification of ν_p requires a closed expression of the solution or at least its structural form and thus is inadequate for a rapid and possibly automated evaluation of large-scale DAE systems (Martinson and Barton, 2000). A concept which is more appropriate for this purpose, is the concept of the differential index ν_d.

2.1.1. The differential index ν_d of DAE systems

The concept of differential index is based on solvability arguments of a linear constant coefficient DAE system $\mathbf{M}\frac{\partial \mathbf{z}}{\partial t} + \mathrm{L}z + \mathbf{u}(t) = \mathbf{0},\ \mathbf{u}(t) \in \mathbb{R}^{n_z}$. Here, $\mathbf{M}, \mathbf{L} \in \mathbb{R}^{n_z \times n_z}$ with constant coefficient matrices $\mathbf{M}, \mathbf{L} \in \mathbb{R}^{n_z \times n_z}$. For these systems the existence and uniqueness of a solution can be shown by transforming the DAE system to into a system of ordinary differential equations (ODE) (Brenan et al., 1996). The number of differentiations required for this transformation, ν_M, is of specific relevance as it can be shown that the following statements hold for $\nu_M > 1$ (Brenan et al., 1996): (i) The number of differential quantities in the DAE system does not correspond to the number of independent initial conditions. (ii) The model formulation implicitly defines additional algebraic relations. These 'hidden' constraints have to be fulfilled by every solution of the DAE system. (iii) The solution of the DAE system depends on $\nu_M - 1$ derivatives of the forcing function $\mathbf{u}(t)$. Thus, for non-smooth forcing, the solution contains discontinuous modes.

The solvability properties of linear constant coefficient DAE systems cannot be generalized to the general nonlinear case. However, it turned out useful to consider this concept in a generalized form, resulting in the differential index ν_d defined as follows:

Definition 2 *(cf. Brenan et al., 1996).* The minimal number of differentiations with respect to time that are to be applied upon all or a subset of the equations of the DAE system $\mathbf{F}\left(\mathbf{z},\ \frac{\partial \mathbf{z}}{\partial t}, \mathbf{u}\right) = \mathbf{0}$ in order to determine $\frac{\partial \mathbf{z}}{\partial t}$ as a continuous function of $\mathbf{z}$ and $\mathbf{u}$ is called the differential index ν_d of the DAE system.

The differential index reflects – in analogy to ν_M – important characteristics of the structure of the equations forming the DAE system. In case a given DAE system is characterized by $\nu_d > 1$, the same problems (i)–(iii) are encountered as for linear DAE systems with $\nu_M > 1$ (Unger et al., 1995).

For nonlinear DAE systems, ν_d can vary locally along the solution trajectory $\mathbf{z}(t)$. A common approach to obtain a global estimate of the differential index for the entire solution space, is the introduction of the structural index ν_s (cf. e.g. Unger et al., 1995; Pantelides, 1988). Whereas the concept of ν_s is based on the definition of ν_d, a conceptually different approach is used in the technical realization of the index analysis. The analyses differ with respect to a qualitative or quantitative evaluation of the dependent variables: In case of ν_d the analysis considers the numerical values of the dependent variables, while in case of ν_s the analysis only considers their structural occurrence. As a result an estimate of a non-local approximation of the differential index is obtained. However, it is to be noted that for specific DAE systems ν_s can strongly differ from ν_d (Reissig et al., 2000).

For a linear constant coefficient DAE the perturbation and differentiation index coincide, i.e. $\nu_p = \nu_d$ (Strehmel, 1992). In the nonlinear case, the differential index possibly underestimates the perturbation index (Campbell and Marszalek, 1999). However, Gear (1990) has shown that the coincidence of ν_d and ν_p also holds for nonlinear semi-explicit DAE systems,

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{y}, \mathbf{u}), \tag{7}$$

$$0 = \mathbf{g}(\mathbf{x}, \mathbf{y}, \mathbf{u}), \tag{8}$$

where the quantities $\mathbf{z}$ and $\mathbf{F}$ have been split up according to $\mathbf{z} = \left[\mathbf{x}^T, \mathbf{y}^T\right]^T$ and $\mathbf{F} = \left[\mathbf{f}^T, \mathbf{g}^T\right]^T$ with $\mathbf{x} \in \mathbb{R}^{n_x}$, $\mathbf{y} \in \mathbb{R}^{n_y}$, $n_x + n_y = n_z$, $\mathbf{f}: \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}^{n_x}$ and $\mathbf{g}: \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}^{n_y}$.

2.1.2. Differential index and consistent initialization

An important problem when working with DAE models is the identification of consistent initial conditions. The consistent initialization problem is best illustrated if the DAE system is considered as an ODE system defined on a manifold in the state space (Rheinboldt, 1984). The dimension and the shape of the manifold is most easily

accessible for semi-explicit DAE systems (7) and (8) of $\nu_d = 1$. Here, the n_y-dimensional manifold can be explicitly represented by

$$M = \{\mathbf{x}, \mathbf{y}, \mathbf{u}(t = t_0) = \mathbf{u}_0 | 0 = \mathbf{g}(\mathbf{x}, \mathbf{y}, \mathbf{u}_0)\}. \tag{9}$$

The ODE system defined on this manifold is then given by Eq. (7).

For this setting it is obvious that the maximal number of independent initial conditions, also referred to as dynamic degrees of freedom (Unger et al., 1995), corresponds to the dimension of the system of underlying ODE. In order to be consistent, these initial conditions are to be specified according to:

Definition 3. The vectors $\mathbf{x}_0$, $\dot{\mathbf{x}}_0$ and $\mathbf{y}_0$ are consistent initial conditions of a DAE system in semi-explicit form with $\nu_d = 1$ if they uniquely solve the DAE system (7) and (8) at $t = t_0$.

The connection of index and consistent initialization gets obvious recalling that in case $\nu_d > 1$ 'hidden' constraints are to be satisfied by any solution of the DAE system. Accordingly, the manifold M associated to the consistent initialization problem is in general not only formed by the explicit algebraic equations but also by the 'hidden' constraints implicitly defined in the DAE system. Thus, the properties – especially the dimension – of the manifold are not directly accessible for a DAE system with $\nu_d > 1$. Hence, in order to identify a consistent set of initial conditions, the algebraic manifold M has to be made explicit. One approach is to apply index reduction to derive an equivalent formulation of the DAE system, which is characterized by $\nu_d = 1$. This way, the manifold (9) is explicitly derived and the consistent initialization problem can be solved according to Definition 3.

An alternative approach for the identification of consistent initial conditions is based on the derivation of an extended system as suggested by Unger et al. (1995).

2.2. Index concepts for PDAE systems

The generalization of the introduced index concepts to PDAE systems have been addressed in numerous works. Before introducing and comparing the resulting generalized concepts, we briefly introduce the formal representation of the PDAE systems considered in this work.

2.2.1. Formal representation of PDAE systems

If not otherwise stated, we refer to PDAE systems defined in the independent variables $\zeta = \{t, x_1, \ldots, x_d\}$, where $t \in [t_0, t_f]$ is time and $x_k \in \left[x_k^L, x_k^U\right]$, $k = 1, \ldots, d$, are the spatial coordinates with appropriate lower and upper bounds. The general structure of a first-order, possibly nonlinear, PDAE system is

$$0 = \mathbf{F}\left(\frac{\partial \omega}{\partial \zeta}, \omega, \mathbf{u}, \mathbf{p}, \zeta\right) \tag{10}$$

with states $\omega(\mathbf{x}, t) \in \mathbb{R}^{n_\omega}$, inputs $\mathbf{u}(t) \in \mathbb{R}^{n_u}$, parameters $\mathbf{p} \in \mathbb{R}^{n_p}$ and state derivatives

$$\frac{\partial \omega}{\partial \zeta} = \left[\frac{\partial \omega}{\partial t}, \frac{\partial \omega}{\partial x_1}, \ldots, \frac{\partial \omega}{\partial x_d}\right]. \tag{11}$$

The system has to be completed by consistent initial and boundary conditions. The consistent specification of initial and boundary conditions will be discussed in Section 4.2.

2.3. Review of index concepts for PDAE systems

PDAE systems differ from DAE systems by a larger number of independent variables. Hence, the generalization of the index concepts from DAE to PDAE systems is generally approached by deriving a transformed system, in which all derivatives of the dependent variables with respect to $n_l - 1$ independent variables are completely determined by the values of the dependent variables themselves. The index is then defined for this transformed system using the same definitions as for DAE system. Hence, in analogy to the DAE case, the conceptually different perturbation and differential indices are distinguished.

In the most simple form, the transformation is based on a MOL approach to discretize the spatial derivatives, e.g., by finite difference or finite element approximations (Campbell and Marszalek, 1996; Weickert, 1996; Sternberg, 2006). Index analysis with respect to time as the only remaining independent variable can then be applied to the semi-discretized system. Campbell and Marszalek (1996) found that the index of the MOL-DAE can be associated with the structural properties of the original PDAE (10). However, it is pointed out that the MOL-based index might depend on the specific domain considered or on the specific spatial discretization method applied.

Following the general concept of semi-discretization, however leaving the actual approximation of the partial derivatives with respect to the spatial coordinates on a more conceptional level, an abstract DAE system is derived from the PDAE system by representing the spatial operators in the form of eigenfunctions (Marszalek and Trzaska, 1995), an orthogonal basis (Campbell and Marszalek, 1999) or a weak formulation (Rang and Angermann, 2005). For this abstract DAE system, a perturbation index with respect to time has been used e.g. in Matthes (2012), Rang and Angermann (2005), Marszalek and Trzaska (1995) and Campbell and Marszalek (1999) to characterize the sensitivity with respect to perturbations in the initial values, boundary conditions and forcing functions. Laplace or Fourier transformations have been used in Campbell and Marszalek (1999), Lucht et al. (1999) and Sternberg (2006) for the introduction of differential indices for specific linear or quasi-linear PDAE systems.

For general, possibly nonlinear, PDAE (10) in n_l independent variables $\zeta = \{\zeta_1, \ldots, \zeta_{n_l}\}$ a conceptually different approach has been introduced by Martinson and Barton (2000) for the definition of differential indices. The approach is motivated by generalizing the consistent initialization problem of DAE systems (cf. Section 2.1.2) to a scenario with n_l independent variables as encountered in PDAE systems. In this context, the authors of Martinson and Barton (2000) consider a $(n_l - 1)$-dimensional hyperplane specified by $\zeta_j = const.$ and $\zeta_i \in \mathcal{I}_i$, $i \in \{1, \ldots, n_l\}$, $i \neq j$, in the n_l-dimensional space spanned by the independent variables. This hyperplane is regarded as a generalization of the zero-dimensional initial point $t = 0$ in the case of a DAE system.

The key element of the index definition is the discrimination of interior and exterior derivatives with respect to a specific hyperplane. Here, the partial derivative $\left.\frac{\partial \omega}{\partial \zeta_j}\right|_{\zeta_j = const.}$ is the (only) exterior derivative; the derivatives $\left.\frac{\partial \omega}{\partial \zeta_i}\right|_{\zeta_j = const.}$, $i \in \{1, \ldots, n_l\}$, $i \neq j$, are interior derivatives. It is important to note that the values of the dependent variables $\omega|_{\zeta_j = const.}$ over the hyperplane completely determine the interior derivatives $\left.\frac{\partial \omega}{\partial \zeta_i}\right|_{\zeta_j = const.}$, $i \in \{1, \ldots, n_l\}$, $i \neq j$. This allows the definition of the differential index with respect to the exterior direction of the hyperplane without the introduction of a detailed concept for the approximation of the interior derivatives as follows:

Definition 5 *(Martinson and Barton, 2000).* The differentiation index with respect to ζ_j, ν_{d,ζ_j}, is the smallest number of times $\mathbf{F}(\cdot)$ in (10) must be differentiated with respect to ζ_j in order to determine $\frac{\partial \omega}{\partial \zeta_j}$ as a continuous function of ω, $\frac{\partial \omega}{\partial \zeta_i}$, $i \in \{1, \ldots, n_l\}$, $i \neq j$, $\mathbf{u}(t)$, $\mathbf{p}$ and ζ_i, $i \in \{1, \ldots, n_l\}$, $i \neq j$.

This definition motivates the characterization of a PDAE system by systematically evaluating the differential indices ν_{d,ζ_j} on all hyperplanes $\zeta_j = const.\, j = 1, \ldots, n_l$. For an analytic or algorithmic index analysis based on Definition 5, a formal representation of the interior derivatives is still needed. The approach used by Martinson and Barton (2000) considers the interior derivatives $\frac{\partial\omega}{\partial\zeta_i}, i \in \{1, \ldots, n_l\}, i \neq j$, as instances of the dependent variable ω itself multiplied with nonzero operator-valued coefficients $\frac{\partial}{\partial\zeta_i}, i \in \{1, \ldots, n_l\}, i \neq j$. The occurrence of these operator-valued coefficients affects the technical realization of an algorithmic analysis of the differential index. However, as shown by Martinson (2000), it does not constrain any symbolic manipulation of equations in the course of the analysis. The concept and algorithms for a structural index analysis (e.g. Unger et al., 1995; Pantelides, 1988) can readily be applied to the pseudo-DAE systems as the corresponding structural representation of the interior derivatives $\frac{\partial\omega}{\partial\zeta_i}, i \in \{1, \ldots, n_l\}, i \neq j$, coincides with the structural representation of the variables ω themselves.

From the different index concepts the approach of Martinson and Barton (2000) stands out as it is applicable to general nonlinear PDAE systems. Further, its relation to consistent initialization of DAE systems makes it useful for the identification of a consistent set of initial and boundary conditions of PDAE systems. Hence, in the remainder of this paper we use Definition 5 and the corresponding theory developed in Martinson and Barton (2000). However, we introduce a formally different nomenclature tailored to PDAE systems in semi-explicit form with respect to all independent variables. As shown in the following, an efficient method for the reduction of the index can be derived for such semi-explicit systems. Further, it can be expected that the differential indices defined in this way are better estimates for the perturbation index, generalizing the reasoning of Gear (1990) and Otter (2014) to the PDAE case.

3. Index analysis and reduction for semi-explicit PDAE systems

This section first introduces the definition of the differential index for PDAE systems cast in semi-explicit pseudo-DAE on hyperplanes. This definition motivates the characterization and – if required – the reformulation of the PDAE system by means of a successive treatment of the pseudo-DAE. Following this idea, we derive a systematic procedure for index analysis and reduction. Before depicting the procedure in detail, the two principal tasks are introduced: (i) index analysis and (ii) index reduction of a pseudo DAE with respect to an independent variable ζ_j.

3.1. Differential index

Following Definition 5, the PDAE system (10) is considered as a set of pseudo-DAE on hyperplanes in the course of the index analysis. However, we require that all n_l pseudo-DAE can be transformed into the semi-explicit form

$$\frac{\partial \mathbf{w}}{\partial \zeta_j} = \mathbf{f}\left(\frac{\partial \mathbf{w}}{\partial \zeta_i}, \mathbf{w}, \frac{\partial \mathbf{y}_1}{\partial \zeta_i}, \mathbf{y}_1, \frac{\partial \mathbf{y}_2}{\partial \zeta_i}, \mathbf{y}_2, \mathbf{u}, \mathbf{p}\right), \tag{12}$$

$$\mathbf{0} = \mathbf{g}\left(\frac{\partial \mathbf{w}}{\partial \zeta_i}, \mathbf{w}, \frac{\partial \mathbf{y}_1}{\partial \zeta_i}, \mathbf{y}_1, \mathbf{u}, \mathbf{p}\right), \quad j, i \in \{1, \ldots, n_l\}, i \neq j, \tag{13}$$

with $\mathbf{w}(\mathbf{x}, t), \mathbf{f} : \mathbb{R}^{n_w} \times \mathbb{R}^{n_w} \times \mathbb{R}^{n_{y_1}} \times \mathbb{R}^{n_{y_1}} \times \mathbb{R}^{n_{y_2}} \times \mathbb{R}^{n_{y_2}} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_w}$ and $\mathbf{y} = \left[\mathbf{y}_1^T, \mathbf{y}_2^T\right]^T, \mathbf{g} : \mathbb{R}^{n_w} \times \mathbb{R}^{n_w} \times \mathbb{R}^{n_{y_1}} \times \mathbb{R}^{n_{y_1}} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_y}, n^\omega = n^w + n^y$. In this form, the model equations are assorted into differential (12) and pseudo-algebraic equations (13) with respect to the independent variable ζ_j. The pseudo-algebraic equation (13) possibly contain partial differential operators $\frac{\partial}{\partial\zeta_i}, i \in \{1, \ldots, n_l\}, i \neq j$. The vector $\mathbf{w}$ comprises the differential quantities with respect to $\zeta_j, j = 1, \ldots, n_l$. All the remaining dependent variables, i.e., the variables for which no derivatives with respect to ζ_j occur, are referred to as pseudo-algebraic variables $\mathbf{y}$. These pseudo-algebraic variables are further distinguished whether they occur only in the differential equations or in both the differential and the pseudo-algebraic equations. According to this criterium the variables are assorted to the vectors $\mathbf{y}_2$ and $\mathbf{y}_1$, respectively.

Example 1 (cont.). The model (3)–(6) corresponds to a PDAE system in the set of independent variables $\zeta = \{t, x\}$. With respect to the independent variable $\zeta_j = t$, it is in semi-explicit form (12) and (13) already, with $\mathbf{w} = [c_A, c_B, c_C, c_D]^T$, $\mathbf{y}_2 = r_1$, $\mathbf{y}_1 = [J_A, J_B, J_C, J_D, r_2]^T$, $\mathbf{u} = v$ and $\mathbf{p} = \left[k, K, s_{k,1}, s_{k,2}\right]^T$. The system can easily be reformulated to a first-order system which is semi-explicit with respect to $\zeta_j = x$. □

For the set of pseudo-DAE (12) and (13) differential indices with respect to all independent variables $\zeta_j, j = 1, \ldots, n_l$ can be defined following Definition 6.

Definition 6 *(Martinson and Barton, 2000).* The differential index ν_{d,ζ_j} with respect to the independent variable ζ_j is defined as the minimal number of differentiations that have to be applied to (12) and (13) or a subset of equations in (12) and (13) to determine $\frac{\partial \mathbf{w}}{\partial \zeta_j}$, $\frac{\partial \mathbf{y}_1}{\partial \zeta_j}$ and $\frac{\partial \mathbf{y}_2}{\partial \zeta_j}$ as continuous functions of $\frac{\partial \mathbf{w}}{\partial \zeta_i}$, $\frac{\partial \mathbf{y}_1}{\partial \zeta_i}$, $\frac{\partial \mathbf{y}_2}{\partial \zeta_i}$, $i = 1, \ldots, n_l \neq j$, $\mathbf{w}$, $\mathbf{y}_2$ and $\mathbf{y}_1$ for given $\mathbf{u}(t)$ and $\mathbf{p}$.

Following Martinson (2000), by introducing operator-valued coefficients for the formal representation of the interior derivatives $\frac{\partial \mathbf{w}}{\partial \zeta_i}$, $\frac{\partial \mathbf{y}_1}{\partial \zeta_i}$ and $\frac{\partial \mathbf{y}_2}{\partial \zeta_i}$, $i \in \{1, \ldots, n_l\}, i \neq j$ the semi-explicit pseudo-DAE system (12) and (13) can be represented as

$$\frac{\partial \mathbf{w}}{\partial \zeta_j} = \bar{\mathbf{f}}(\mathbf{w}, \mathbf{y}_1, \mathbf{y}_2, \mathbf{u}, \mathbf{p}), \tag{14}$$

$$\mathbf{0} = \bar{\mathbf{g}}(\mathbf{w}, \mathbf{y}_1, \mathbf{u}, \mathbf{p}), \quad j = 1, \ldots, n_l, \tag{15}$$

with $\bar{\mathbf{f}} : \mathbb{R}^{n_w} \times \mathbb{R}^{n_{y_1}} \times \mathbb{R}^{n_{y_2}} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_w}$ and $\bar{\mathbf{g}} : \mathbb{R}^{n_w} \times \mathbb{R}^{n_{y_1}} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_y}$.

3.2. Index analysis

The criterion for the pseudo-DAE system (14) and (15) to be of index $\nu_{d,\zeta_j} > 1$ is

$$\det\left(\frac{\partial \bar{\mathbf{g}}(\mathbf{w}, \mathbf{y}_1, \mathbf{u}, \mathbf{p})}{\partial \mathbf{y}_1}\right) = 0. \tag{16}$$

It expresses the fact that the pseudo-algebraic variables $\mathbf{y}_1$ are not uniquely determined by the set of pseudo-algebraic equations, i.e., the set of equations (15) is structurally singular with respect to $\mathbf{y}_1$.

In many cases, the structural singularity of the pseudo-algebraic equations (15), and thus the high-index behavior, is caused by a subsystem of pseudo-algebraic equations

$$\mathbf{0} = \Omega_{\zeta_j}(\mathbf{w}, \mathbf{y}_1, \mathbf{u}, \mathbf{p}), \tag{17}$$

of (15) with $\Omega_{\zeta_j} : \mathbb{R}^{n_w} \times \mathbb{R}^{n_{y_1}} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_{\Omega_{\zeta_j}}}, n_\Omega \leq n_y$. Formally, such a subsystem, – referred to as minimal structurally singular subsystem (MSSS) – is defined as the smallest subsystem of the pseudo-algebraic equations (15) which is structurally singular (Neumann, 2004), i.e. which has the property

$$\det\left(\frac{\partial \Omega_{\zeta_j}(\mathbf{w}, \tilde{\mathbf{y}}_1, \mathbf{u}, \mathbf{p})}{\partial \tilde{\mathbf{y}}_1}\right) = 0 \tag{18}$$

for any pseudo-algebraic variables $\tilde{\mathbf{y}}_1$ taken from $\mathbf{y}_1$ with $dim(\tilde{\mathbf{y}}_1) \leq dim(\mathbf{y}_1)$ and $dim(\tilde{\mathbf{y}}_1) \leq n_\Omega$ (Neumann, 2004). Due to this property, the MSSS couples differential quantities by algebraic constraints. An important special case where this coupling is obvious is the MSSS

$$\mathbf{0} = \Omega_{\zeta_j}(\mathbf{w}, \mathbf{u}, \mathbf{p}). \tag{19}$$

As (19) does not show any dependence on $\tilde{\mathbf{y}}_1$, criterion (18) is trivially fulfilled.

Example 1 (cont.). Consider the pseudo-DAE system with respect to $\zeta_j = t$ of the tubular reactor model (3)–(6). Obviously, criterion (16) is fulfilled and the algebraic equation (5) forms the scalar MSSS

$$\Omega_t = K - \frac{c_A\, c_B}{c_C}. \tag{20}$$

Correspondingly, we find $\nu_{d,t} > 1$. A similar result is obtained for reformulation of Eqs. (3)–(6) to a pseudo-DAE system with respect to x. A MSSS is again formed by (5) and correspondingly $\nu_{d,x} > 1$. □

3.3. Generalization of the index reduction algorithm

The procedure for a systematic index reduction that is used here is based on the work of Asbjørnsen (Asbjørnsen and Fjeld, 1970) and Bachmann (Bachmann et al., 1990). It corresponds to an extension of the algorithm proposed by Moe (1995) for the index reduction of DAE systems to PDAE systems. Further, we modify the algorithm by tailoring it to the concept of MSSS causing the structural singularity. The latter improves the method significantly, as not all algebraic equations have to be used in the reformulation procedure.

The basis for the reduction procedure is to exploit the fact that an MSSS (17) is characterized by its structural singularity with respect to the pseudo-algebraic variables $\tilde{\mathbf{y}}_1$. If (17) is differentiated with respect to ζ_j, it is obvious that also the differentiated MSSS

$$0 = \frac{\partial \Omega_{\zeta_j}}{\partial \zeta_j} = \frac{\partial \Omega_{\zeta_j}}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \zeta_j} + \frac{\partial \Omega_{\zeta_j}}{\partial \mathbf{y}_1} \frac{\partial \mathbf{y}_1}{\partial \zeta_j} + \frac{\partial \Omega_{\zeta_j}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \zeta_j} \tag{21}$$

does not determine $\frac{\partial \tilde{\mathbf{y}}_1}{\partial \zeta_j}$ uniquely. Eq. (21) can be rewritten as an underdetermined linear system

$$\mathbf{A} \frac{\partial \tilde{\mathbf{y}}_1}{\partial \zeta_j} = \mathbf{b} \tag{22}$$

with

$$\mathbf{A} = \frac{\partial \Omega}{\partial \tilde{\mathbf{y}}_1} \in R^{n_\Omega \times n_{\tilde{y}_1}}, \quad \mathbf{b} = -\frac{\partial \Omega}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \zeta_j} - \frac{\partial \Omega}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \zeta_j} \in R^{n_\Omega}. \tag{23}$$

Note that $\frac{\partial \mathbf{w}}{\partial \zeta_j}$ is given by Eq. (14) and $\frac{\partial \mathbf{u}}{\partial \zeta_j}$ is the derivative of the known inputs $\mathbf{u}$ and thus a known function itself. Hence, $\mathbf{b}$ corresponds to a quasi-linear combination of the righthand side of the differential equations and the derivatives of the inputs. A necessary solvability condition for Eq. (22) is

$$\Gamma^T \mathbf{b} = 0. \tag{24}$$

Here Γ is a matrix of basis vectors of the nullspace of $\mathbf{A}^T$ (Moe, 1995), which is defined as the set of linear independent vectors $\{\gamma_1, \ldots, \gamma_{n_n}\}$, $n_n = n_\Omega - \text{rank}(\mathbf{A})$ satisfying

$$\mathbf{A}\gamma_i = 0, \quad i = 1, \ldots, n_n. \tag{25}$$

If the MSSS has the form (19), $\mathbf{A} = \frac{\partial \Omega}{\partial \tilde{\mathbf{y}}_1}$ is not properly defined. For this particular case we define $\Gamma = \mathbf{I}$ with $\mathbf{I} \in \mathbb{R}^{n_{\Omega_{\zeta_j}}}$ as the unity matrix.

The criterion (24) together with (23) reveals an additional system of equations

$$\Gamma^T \mathbf{b} = \mathbf{g}_{add,\zeta_j}(\mathbf{w}, \mathbf{y}_1, \mathbf{u}, \mathbf{p}) = 0, \tag{26}$$

linking differential and algebraic variables of the model, which every solution of the PDAE system has to fulfill. The differential index of the pseudo-DAE systems (14) and (15), can be reduced, if the additional constraints (26) are used to substitute the corresponding number of differential equations. As (26) corresponds to quasi-linear combinations of the original model equations, this procedure preserves the physical information of the original formulation.

Example 1 (cont.). The index reduction method is applied to the high-index model of the tubular reactor. First, we consider the pseudo-DAE with respect to $\zeta_j = t$. Symbolic differentiation of the MSSS (20) yields

$$\frac{\partial \Omega_t}{\partial \mathbf{w}} = [\, -c_B \quad -c_A \quad K \quad 0\,], \tag{27}$$

and, as $\frac{\partial \Omega_t}{\partial \mathbf{u}} = 0$, (23) is evaluated to

$$b = -c_B \left(-\frac{\partial J_A}{\partial x} - \nu \frac{\partial c_A}{\partial x} - r_1 \right) - c_A \left(-\frac{\partial J_B}{\partial x} - \nu, \frac{\partial c_B}{\partial x} - r_1 - r_2 \right) + K \left(-\frac{\partial J_C}{\partial x} - \nu \frac{\partial c_C}{\partial x} + r_1 \right). \tag{28}$$

Note that the convective terms in (28) comprising first derivatives with respect to x cancel out, because

$$\frac{\partial \Omega_t}{\partial x} = K \frac{\partial c_C}{\partial x} - c_A \frac{\partial c_B}{\partial x} - c_B \frac{\partial c_A}{\partial x} = 0. \tag{29}$$

As the MSSS (20) is of the form (19), the nullspace is defined as $\Gamma = 1$. Thus, the additional constraint

$$g_{add,t} = c_B \frac{\partial J_A}{\partial x} + c_A \frac{\partial J_B}{\partial x} - K \frac{\partial J_C}{\partial x} + r_1 (c_A + c_B + K) + c_A r_2 = 0 \tag{30}$$

is obtained as a quasi-linear combination of the original species balance equations (3). If one of the species balance equations (3) – for instance the one of species A – is substituted by Eq. (30), a reformulated system of $\nu_{d,t} = 1$ is obtained. As one differentiation has been applied in the course of the index-reduction, the differential index of the original model (3)–(6) with respect to time is $\nu_{d,t}^{orig} = 2$. □

3.4. Systematic procedure for the index analysis and reduction

Based on the concepts and procedures introduced above, we propose a systematic procedure for the index analysis and reduction of PDAE systems as illustrated in algorithm. It starts with a given model in the form of a PDAE system in the independent variables $\zeta_1, \ldots, \zeta_{n_l}$. In step 4 of the procedure a first-order pseudo-DAE is formulated with respect to the first independent variable ζ_1. For this system, the differential index ν_{d,ζ_1} is calculated in step 5 using the framework introduced in Section 3.2. In case $\nu_{d,\zeta_1} > 1$, the model is reformulated in the steps 7-9 using the index reduction described in Section 3.3. This yields a reformulated model which is subject to another index analysis in step 11. The index reduction process is successively carried out until a reformulated model is obtained that is characterized by $\nu_{d,\zeta_1} = 1$. From the number of times the index reduction procedure has been applied, which is equivalent to the number of differentiations $n_{diff,j}$ applied to the model, the index $\nu_{d,j}^{orig}$ is calculated in step 13. Then the procedure is restarted in step 3 for the next independent variable ζ_2. The procedure terminates after sequentially going through each independent variable $\zeta_j \in \zeta$.

Algorithm. Index reduction algorithm for PDAE systems

1 formulate PDAE system in the general form Eq. (10) in the independent variables $\zeta_1, \ldots, \zeta_{n_l}$
2 **for** $j = 1, \ldots, n_l$ **do**
3 reformulate the PDAE system as a pseudo-DAE with respect to ζ_j in the form (14) and (15)
4 **analyze** if $\nu_{d,\zeta_j} > 1$ by evaluating (16)
5 **set** $n_{diff,j} = 0$ `/* init. number of differentiations */`
6 **while** $\nu_{d,\zeta_j} > 1$ **do**
7 **identify** the MSSS Ω_{ζ_j}
8 **apply** systematic index reduction as described in Section 3.3
9 **set** $n_{diff,j} = n_{diff,j} + 1$
10 **analyze** if $\nu_{d,\zeta_j} > 1$ by evaluating (16)
11 **end while**
12 **set** $\nu_{d,j}^{orig} = n_{diff,j} + 1$ `/* calc. index of original model */`
13 **end for**

Example 1 (cont.). The procedure is illustrated by considering the tubular reactor model, where we can use the results obtained in the previous sections. Thus, we already found the results for steps 1–9 in algorithm for $\zeta_j = t$: The index of the original modeling equations with respect to time is $\nu_{d,t} > 1$. The index reduction procedure identifies the additional constraint (30) which is used to eliminate one of the original balance equations, e.g., the balance equation for species A. As the resulting reformulated model is characterized by $\nu_{d,t} = 1$, the method exits the index-reduction loop and determines the index of the original model $\nu_{d,t}^{orig} = 2$. The method continues by considering the next independent variable in ζ, i.e., $\zeta_j = x$. Hence, consider the model of the tubular reactor after its reformulation in the index reduction process with respect to time t. This reformulated model is expressed as a first-order system in semi-explicit form with respect to x as

$$\frac{\partial J_k}{\partial x} = -\frac{\partial c_k}{\partial t} + \nu \frac{J_k}{D^{ax}} + s_{k,1} r_1 + s_{k,2} r_2, \quad k \in \{B, C, D\}, \tag{31}$$

$$\frac{\partial J_A}{\partial x} = -\frac{c_A}{c_B}\left(-\frac{\partial c_B}{\partial t} + \nu \frac{J_B}{D^{ax}} - r_1 - r_2\right) + \frac{K}{c_B}\left(-\frac{\partial c_C}{\partial t} + \nu \frac{J_C}{D^{ax}} + r_1\right) - \frac{1}{c_B} r_1 (c_A + c_B + K) - \frac{1}{c_B} r_2 c_A, \tag{32}$$

$$\frac{\partial c_k}{\partial x} = -\frac{J_k}{D^{ax}}, \quad k \in \{A, B, C, D\}, \tag{33}$$

$$0 = K - \frac{c_A c_B}{c_C}, \tag{34}$$

$$0 = r_2 - k c_B, \tag{35}$$

using (3), (30) and (4)–(6). The index analysis of (31)–(35) with respect to x in step 5 reveals $\nu_{d,x} > 1$ and a MSSS is formed by

$$\Omega_x = K c_C - c_A c_B = 0 \tag{36}$$

Thus, the mass-action law (34) imposes again a "hidden" constraint implicitly relating the fluxes of species A, B and C. The algorithm continues in step 9 with the index reduction of the pseudo-DAE with respect to x. In this process, symbolic differentiation yields

$$\frac{\partial \Omega_{x,1}}{\partial w} = \begin{bmatrix} 0 & 0 & 0 & 0 & -c_B & -c_A & K & 0 \end{bmatrix}. \tag{37}$$

Noting that the MSSS (36) is in the form (19), which implies $\Gamma = 1$, (23) and (26) give the additional constraint

$$g_{add,x} = c_B J_A + c_A J_B - K J_C = 0, \tag{38}$$

as a quasi-linear combination of constitutive equations (33) for the dispersive fluxes of the species that are involved in the equilibrium reaction A, B and C. To reduce the index of the model (31)–(35), Eq. (38) is used to substitute one constitutive equation of the dispersive fluxes (33), e.g., of species A. Note that, due to this substitution, c_A becomes an algebraic quantity in the reformulated model, i.e. in the reformulated model we find $\mathbf{w} = [J_A, J_B, J_C, J_D, c_B, c_C, c_D]^T$, $\mathbf{y}_1 = [c_A, r_1]^T$ and $\mathbf{y}_2 = [r_2]^T$.

The method continues in step 11 carrying out an index analysis of the reformulated model. The analysis reveals that the reformulated model is still characterized by $\nu_{d,x} > 1$. Correspondingly, another index reduction step is required. The MSSS inducing the high-index behavior is formed by the algebraic equations (34) and (38), i.e.,

$$\Omega_x = \begin{bmatrix} c_B J_A + c_A J_B - K J_C \\ K c_C - c_A c_B \end{bmatrix} = 0. \tag{39}$$

Symbolic differentiation yields

$$\frac{\partial \Omega_x}{\partial \mathbf{w}} = \begin{bmatrix} c_B & c_A & -K & 0 & J_A & 0 & 0 \\ 0 & 0 & 0 & 0 & -c_A & K & 0 \end{bmatrix}. \tag{40}$$

With this Eq. (23) can be evaluated by multiplying Eq. (40) from the right with the right-hand side of the differential equations $\mathbf{f}(\mathbf{w}, \mathbf{y}_1, \mathbf{y}_2, \mathbf{u}, \mathbf{p})$ and symbolic reformulation yielding

$$\frac{\partial \Omega_{x,2}}{\partial \mathbf{w}} \mathbf{f}(\mathbf{w}, \mathbf{y}_1, \mathbf{y}_2, \mathbf{u}, \mathbf{p}) = \begin{bmatrix} -r_1(c_A + c_B + K) - r_2 c_A - \frac{J_A J_B}{D^{ax}} \\ c_A \frac{J_B}{D^{ax}} - K \frac{J_C}{D^{ax}} \end{bmatrix}. \tag{41}$$

The algebraic variables in the MSSS (39) are $\tilde{\mathbf{y}}_1 = [c_A]$. Thus, we obtain from (23)

$$\mathbf{A} = \begin{bmatrix} J_B \\ -c_B \end{bmatrix}. \tag{42}$$

According to (25), a basis for the nullspace of $\mathbf{A}^T$ is formed by

$$\Gamma = \begin{bmatrix} \frac{1}{J_B} & \frac{1}{c_B} \end{bmatrix}^T, \tag{43}$$

which is used to finally derive the additional constraint by evaluating Eq. (26),

$$g_{add,x} = -r_1 c_B D^{ax}(c_A + c_B + K) + r_2 c_B c_A D^{ax} - 2 c_B J_B J_A = 0. \tag{44}$$

This second additional constraint (44) derived in the reduction with respect to x can be used to substitute one differential equation that has been used in the reformulation process, i.e., all differential equations except the species balance (31) and definition of the dispersive flux (33) for species D. By choosing (32), the reformulated model

$$\frac{\partial c_k}{\partial t} = -\frac{\partial J_k}{\partial x} - \nu \frac{\partial c_k}{\partial x} + s_{k,1} r_1 + s_{k,2} r_2, \quad k \in \{B, C, D\}, \tag{45}$$

$$J_k = -D^{ax} \frac{\partial c_k}{\partial x}, \quad k \in \{B, C, D\}, \tag{46}$$

$$0 = -r_1 c_B D^{ax}(c_A + c_B + K) + r_2 c_B c_A D^{ax} - 2 c_B J_B J_A, \tag{47}$$

$$0 = c_B J_A + c_A J_B - K J_C, \tag{48}$$

$$0 = K - \frac{c_A c_B}{c_C}, \tag{49}$$

$$0 = r_2 - k c_B, \tag{50}$$

is obtained. The next step of the procedure, step 11, is the index analysis of the reformulated model (45)–(50), which yields $\nu_{d,x} = 1$. As in total two differentiations have been carried out upon the mass-action-law (49), the index of the original model formulation is $\nu_{d,x}^{orig} = 3$.

As x is the last independent variable in ζ the method terminates at this point, providing the reformulated model, information concerning the indices of the original model formulation, $\nu_{d,t} = 2$ and $\nu_{d,x} = 3$ as well as information concerning invariants of the system explicit in the additional constraints (47) and (48).

4. Index analysis and reduction in the modeling work-flow

In this section, we illustrate the relevance of the systematic index analysis and reduction procedure in a modeling work-flow for distributed models. In Section 4.1 it is shown how the results of the proposed method support the physical interpretation of the model. With respect to the evaluation of the consistency of initial and boundary conditions we discuss in Section 4.2 the benefits and the limitations of the results obtained from the method.

4.1. Physical interpretation of the reformulated model

The index analysis of a DAE system provides important information on its dynamic degrees of freedom (cf. Section 2.1.2) corresponding to the maximal number of independent initial conditions. Next to the specification of initial conditions, the dynamic degrees of freedom constitute an important model property with respect to its physical interpretation. Most important in this context is the coincidence between the dynamic degrees of freedom and the number of model states independently describing extensive quantities in the model. Thus, if we assume that the system is described correctly by the model, the dynamic degrees of freedom can help to identify the number of extensive quantities in the physical system that are truly independent. The other way round, if the number of independent extensive quantities is known, e.g., by theoretical considerations or experiments, the dynamic degrees of freedom give a criterion to evaluate the potential of the model to describe the underlying relations correctly.

The concept of dynamic degrees of freedom for DAE can be generalized to PDAE systems in a straightforward manner. The key aspect allowing this generalization, is the definition of the differential index for semi-explicit pseudo-DAE systems (14) and (15). If the pseudo-DAE with respect to the independent variable ζ_j is characterized by $\nu_{d,j} = 1$, the dimension of the differential system (14) directly provides the number of truly independent differential quantities with respect to ζ_j. For this measure, we introduce the notion of differential degrees of freedom with respect to an independent variable ζ_j as follows:

Definition 7. For a given pseudo-DAE with respect to ζ_j, (14) and (15), characterized by $\nu_{d,j} = 1$, the differential degrees of freedom $d_{f,j}$ with respect to ζ_j correspond to the dimension of the differential system (14).

According to this definition the differential degrees of freedom are a direct result of the procedure for the systematic index analysis and reduction to pseudo-DAE systems characterized by $\nu_{\zeta_j} = 1$.

Example 1 (cont.). If the reformulated model (45)–(50) is expressed as a pseudo-DAE with respect to time in the form (14) and (15), the differential subsystem (14) has the dimension three, i.e. we find $d_{f,t} = 3$. Hence, the reformulated model shows explicitly that the dynamics of the system are governed by three differential states with respect to time. In this context, the four holdup terms $\frac{\partial c_i}{\partial t}$, $i \in \{A, B, C, D\}$ in the original model formulation (3)–(6) apparently give a misleading picture of the physics described by the PDAE system. The same holds true for the independent differential states with respect to x. Here, we find $d_{f,x} = 6$. Hence, not eight as suggested by the original model formulation (3)–(6), but six independent differential states with respect to x are encountered.

In addition to the differential degrees of freedom, the index reduction method provides further insight into physically relevant model properties. These properties are found in the invariant expressions with respect to certain independent variables revealed as additional constraints in the index reduction. In many cases, it is even possible to obtain a physical interpretation of these invariants highlighting important physical principles that are depicted in the model. Assuming that the model describes the underlying physical phenomena correctly, the revealed physical principles contribute to a better understanding of the phenomena themselves. This gain of physical insight is illustrated next as well as in further examples given in Section 5.

Example 1 (cont.). The index reduction with respect to time reveals the additional constraint (47) by means of a quasi-linear combination of the original species balance equations. From a technical point of view, this is achieved by lumping the holdup terms $\frac{\partial c_k}{\partial t}$, $k \in \{A, B, C, D\}$, into the term $\frac{\partial}{\partial t}\left(\frac{c_A c_B}{c_C}\right)$, which is characterized by an invariant behavior with respect to time. The invariance of the quotient $\frac{c_A c_B}{c_C}$ is revealed in an analogous manner in the index reduction with respect to the spatial coordinates. Hence, only three of the dispersive fluxes $J_k \in k \in \{A, B, C, D\}$ defined in (4) are independent.

Here, it is interesting to recall that the constitutive equations (4) correlate the dispersive fluxes to their driving forces, which are the concentration gradients. In this context, the derivation of the additional constraint (38) illustrates that only three of the four driving forces are independent in order to preserve the chemical equilibrium imposed by the mass action law (49).

4.2. Identification of consistent initial and boundary conditions

The PDAE model equations have to be completed by a consistent set of initial and boundary conditions. From a technical point of view, the specification targets at obtaining a complete problem formulation that matches a specific physical scenario, e.g. specific concentrations in the reaction media at $t = t_0$ or a free outflow at the end of the tubular reactor. From a mathematical perspective, the specified initial and boundary conditions represent additional data that either (i) select a unique member of a set of solutions or (ii) construct the functional form of the solution. In the former case, it is referred to as a restricted solution (Martinson, 2000) while in the latter case it is referred to as an unrestricted solution. To accomplish this role, the set of initial and boundary data has to be in agreement with specific criteria, i.e., it has to be consistent to yield a well-posed problem.

A closed theory and appropriate methods for testing the consistency of initial and boundary conditions for a general PDAE system is still missing. However, the procedure for the index reduction provides valuable information to support the consistent specification of initial and boundary conditions: The number of differential degrees of freedom with respect to a time $d_{f,t}$ corresponds to the maximal number of initial conditions n^{IC} that can be specified independently. Further, the results of the method support the analysis of the consistency of the initial conditions, as the resulting pseudo-DAE with respect to time is characterized by $\nu_{d,t} = 1$ and is in semi-explicit form (14) and (15). Hence, Definition 3 can be generalized to the pseudo-DAE in a straightforward manner. Accordingly, the initial conditions in combination with the model equations (14) and (15) have to uniquely determine the algebraic variables $\mathbf{y}|_{t=t_0}$, the differential variables $\mathbf{w}|_{t=t_0}$ and their gradients $\left.\frac{\partial \mathbf{w}}{\partial t}\right|_{t=t_0}$ on the hyperplane $t = t_0$.

The number of differential degrees of freedom with respect to a spatial coordinate corresponds to the total number of boundary conditions $n_{BC,x_k} = n_{BC,x_k^U} + n_{BC,x_k^L}$ that can be specified

independently at the upper or lower bounds of the coordinate x_k, x_k^U and x_k^L.

Example 1 (cont.). The number of differential degrees of freedom with respect to time is $d_{f,t} = 3$; hence, $n^{IC} = 3$ initial conditions have to be specified. The specification of four initial conditions as suggested by the four differential states in the original model formulation would easily result in inconsistent initial conditions and thus in a badly posed problem. The initial conditions

$$c_k(t = 0, x) = c_{k,0}(x) k \in \{B, C, D\}, \tag{51}$$

and the reformulated model (45)–(50) uniquely determine the algebraic variables $\mathbf{y} = \mathbf{y}_1 = [J_A, J_B, J_C, J_D, c_A, r_1, r_2]^T$, the differential variables $\mathbf{w} = [c_B, c_C, c_D]^T$ and their gradients $\frac{\partial \mathbf{w}}{\partial t}\Big|_{t=t_0} = \left[\frac{\partial c_B}{\partial t}\Big|_{t=t_0}, \frac{\partial c_C}{\partial t}\Big|_{t=t_0}, \frac{\partial c_D}{\partial t}\Big|_{t=t_0}\right]$ on the hyperplane $t = t_0$.

Concerning the consistent specification of boundary conditions, the work-flow reveals the total number of boundary conditions that can be specified independently as $n_{BC,x} = d_{f,x} = 6$. The specification of eight boundary conditions as suggested by the original model formulation is typically inconsistent.

No information is provided by the proposed procedure concerning the distribution of the specified boundary conditions to the lower or upper bound of the spatial coordinates. Hence, additional information has to be added to evaluate the consistency of the boundary conditions. In the case of a linear PDAE system, a comprehensive theory for the consistent specification of boundary conditions has been developed by Martinson and Barton (2003). These authors derive criteria for the well-posedness of a given specification of initial and boundary conditions by generalizing characteristic analysis of hyperbolic PDE to general PDAE systems. The essence of the method is to use a block decomposition method to transform the system into a canonical form. In this form, the resulting block rows can be distinguished by showing either hyperbolic, parabolic or differential characteristics. According to the characteristics, the boundary conditions are to be specified at the upper or lower boundary of the domain.

However, in addition to its restriction to linear PDAE systems, the method has two major limitations: (i) PDAE systems are considered which are characterized by an unrestricted solution and (ii) the theory only holds for $n_l = 2$ and cannot be generalized to higher-dimensional PDAE systems. Hence, PDAE systems classified as ill-posed according to the results of the characteristic analysis can be well-posed if they are considered as restricted problems. A particular example of the latter case is the well-known heat equation (Martinson and Barton, 2003).

For general PDAE systems, methods for investigating the consistency of a given specification of boundary conditions are typically system-specific and require a high level of expertise. A particular exception is the evaluation of the consistency for specific standard types of PDAE systems. Hence, a useful approach to characterize a given PDAE system is to apply explicit transformations to yield a reformulated system in standard form.

Example 1 (cont.). In this particular example, information for a consistent specification of boundary conditions is obtained by the elimination of the algebraic variables $\mathbf{y}$ by substitution of (46)–(50) into (45). This yields a system of second-order reaction-diffusion equations which are known to be parabolic. Thus, the boundary conditions are to be equally distributed to the upper and lower bounds of x, e.g., in the form of the well-known Danckwerts boundary conditions (Danckwerts, 1995)

$$v\, c_{k,x_L}(t) = v\, c_k(t, x = x_L) - D^{ax} \frac{\partial c_k}{\partial x}\Big|_{x=x_L}, \tag{52}$$

$$\frac{\partial c_k}{\partial x}\Big|_{x=x_U} = 0, \quad k \in \{B, C, D\}. \tag{53}$$

5. Applications of the proposed procedure

The proposed procedure for index analysis and reduction is applied in the context of the modeling work-flow for two modeling problems to illustrate its capabilities and limitations. First, the diffusive transport of ionic species at infinite dilution is considered. The second model considered is the well-known Navier–Stokes system for incompressible fluid flows.

5.1. Diffusive transport in liquid electrolyte mixture

The transport of n ionic species in a liquid electrolyte is described by the PDAE system

$$\frac{\partial c_k}{\partial t} = -\nabla \cdot \mathbf{J}_k - \nabla \cdot (\mathbf{v}\, c_k), \quad k = 1, \ldots, n, \tag{54}$$

$$\mathbf{J}_k = -D_k \nabla c_k + \frac{z_k c_k}{RT} D_k F\, \mathbf{E}, \quad k = 1, \ldots, n, \tag{55}$$

$$\mathbf{E} = -\nabla \phi, \tag{56}$$

$$0 = \sum_{k=1}^{n} z_k c_k. \tag{57}$$

The scenario of an infinitely diluted isothermal solution is considered, so that the species balance equation for the solvent is trivially fulfilled and the transport processes do not affect the velocity of the solvent $\mathbf{v}$. To simplify the problem, $\mathbf{v}$ is considered as a known input, e.g., provided by a possibly analytical solution of the Navier–Stokes equation (cf. Section 5.2). Next to the n species balance equations (54), the Nernst–Planck equations (55) are introduced to describe the flux densities $\mathbf{J}_k$ of ionic species as a superposition of transport induced by diffusion and by the electric field $\mathbf{E}$. Eq. (56) defines the electric field $\mathbf{E}$ as the negative gradient of the electric potential ϕ (Kontturi et al., 2008). The algebraic equation (57) corresponds to the well-known electroneutrality condition (Newman and Thomas-Alyea, 2004) enforcing a local space charge of zero. c_k is the volumetric concentration, D_k is the diffusion coefficient and z_k is the charge number of species k. The Faraday constant F, the gas constant R and the temperature T are constant model parameters.

5.1.1. Index analysis and reduction

We continue with the reformulation in step 4 of the algorithm, which is trivial, since the model (54)–(57) is in semi-explicit form with respect to time. In step 5, the index is analyzed, yielding $\nu_{d,t} > 1$.

The succeeding index reduction in steps 7–10 reveals the additional constraint

$$g_{add,t} = -\sum_{k=1}^{n} z_k \nabla \cdot \mathbf{J}_k = 0. \tag{58}$$

This constraint is used to substitute the species balance equation (54) for any species in the solution to reduce the index, the first species $k = 1$ for example. The method continues in step 11 to analyze the index of the reformulated model. As this can be characterized by $\nu_{d,t} = 1$, the index of the original model with respect to time is $\nu_{d,t}^{orig} = 2$. The method returns to step 4 in order to obtain a PDAE system in semi-explicit form with respect to the next independent variable, i.e. x_1, by symbolic manipulation. In step 5 the analysis reveals that the index of the reformulated model with

respect to x_1 is larger than one. The index reduction method applied in the steps 7–10 yields the additional constraint

$$g_{add,x_1} = -\sum_{k=1}^{n} z_k \frac{J_{x_1,k}}{D_k} + \sum_{k=1}^{n} \frac{z_k^2 c_k}{RT} F E_{x_1} = 0, \tag{59}$$

where $J_{x_1,k}$ and E_{x_1} are the scalar entries of the flux density $\mathbf{J}_k$ and electric field $\mathbf{E}$ vectors in the x_1-direction. To reduce the index ν_{d,x_1}, the constraint (59) is used to substitute one scalar element of the vectorial Nernst–Planck equation (55) for any species in the set of species, e.g., for the first species

$$J_{x_1,1} = -D_1 \nabla c_1 + \frac{z_1 c_1}{RT} D_1 F E_{x_1}. \tag{60}$$

The method continues in step 11 to analyze the index of the reformulated model yielding $\nu_{d,x_1} = 1$. Thus, the index of the original formulation with respect to x_1 is $\nu_{d,x_1}^{orig} = 2$. In the next few steps the method is continued by analyzing and reducing the index with respect to the remaining independent variables x_2 and x_3. As the model is symmetric in the spatial coordinates, it is conclusive that the method in an analogous manner identifies the high-index behavior and reveals additional constraints similar to Eq. (59) for x_2 and x_3. In vectorial notation these three scalar additional constraints obtained in the reduction process with respect to x_1, x_2 and x_3 are expressed as

$$\mathbf{g}_{add,\mathbf{x}} = -\sum_{k=1}^{n} z_k \frac{\mathbf{J}_k}{D_k} + \sum_{k=1}^{n} \frac{z_k^2 c_k}{RT} F \mathbf{E} = 0. \tag{61}$$

For the reduction of the index with respect to all spatial coordinates (61) is used to substitute the vectorial Nernst–Planck equation (55) of the first species. As a final result, the method yields the reformulated model

$$\frac{\partial c_k}{\partial t} = -\nabla \cdot \mathbf{J}_k - \nabla \cdot (\mathbf{v} c_k), \quad k = 2, \ldots, n, \tag{62}$$

$$0 = -\sum_{k=1}^{n} z_k \nabla \cdot \mathbf{J}_k, \tag{63}$$

$$\mathbf{J}_k = -D_k \nabla c_k + \frac{z_k c_k}{RT} D_k F \mathbf{E}, \quad k = 2, \ldots, n, \tag{64}$$

$$0 = -\sum_{k=1}^{n} z_k \frac{\mathbf{J}_k}{D_k} + \sum_{k=1}^{n} \frac{z_k^2 c_k}{RT} F \mathbf{E}, \tag{65}$$

$$\mathbf{E} = -\nabla \phi, \tag{66}$$

$$0 = \sum_{k=1}^{n} z_k c_k, \tag{67}$$

and the indices of the original model formulation $\nu_{d,t} = 2$ and $\nu_{d,x_j} = 2,\ j = 1, \ldots, 3$.

5.1.2. Physical interpretation and consistent initial and boundary conditions

The reduction process and the additional constraints (63) and (65) reveal important physical principles tacitly represented in the model. In the first reduction step, the lumped storage term $\frac{\partial \sum_{k=1}^{n} z_k c_k}{\partial t}$ is formed as a linear combination of the original storage terms $\frac{\partial c_k}{\partial t}$, $k = 1, \ldots, n$, highlighting the invariance of the volumetric space charge $\rho^e = F \sum_{k=1}^{n} z_k c_k = 0$. To express this explicitly in the model, the method derives Eq. (63) as a linear combination of the species balance equations (54). By introducing the definition of the current density (Newman and Thomas-Alyea, 2004)

$$\mathbf{i} = F \sum_{k=1}^{n} z_k \mathbf{J}_k, \tag{68}$$

it becomes obvious that (63) corresponds to the stationary charge balance

$$0 = \nabla \cdot \mathbf{i}. \tag{69}$$

The invariance of the charge density with respect to the spatial coordinates is expressed in the constraint (65). In analogy to the tubular reactor model illustrated in the example, the number of independent driving forces for the diffusive transport is $n-1$ rather than n suggested by the original model. Further, it is interesting to note that the constraint (65) gives an implicit algebraic relation between the current density and the electric field as a generalization of Ohm's law, i.e.,

$$\mathbf{i} = \kappa \mathbf{E}. \tag{70}$$

It can easily be verified that (65) really corresponds to the generalization of (70), if a scenario with equal diffusion coefficients $D_k = \tilde{D}$, $k = 1, \ldots, n$, is considered and the local conductivity of the solution is introduced as $\kappa = \sum_{k=1}^{n} \frac{z_k^2 c_k}{RT} \tilde{D} F$ (cf. Newman and Thomas-Alyea, 2004).

The reformulated model has $d_{f,t} = n-1$ differential degrees of freedom with respect to time so that in total $n^{IC} = n-1$, rather than n, initial conditions can be specified independently. A natural choice would be the specification of $n-1$ initial concentrations

$$c_k(t = 0, \mathbf{x}) = c_{k,0}(\mathbf{x}), \quad k = 2, \ldots, n. \tag{71}$$

The identification of a consistent set of boundary conditions is more involved. However, the reformulated model provides an adequate basis for investigating this question. The differential degrees of freedom with respect to the spatial coordinates are determined as $d_{f,x_k} = 2n$, $k = 1, \ldots, 3$. Hence, in total $n_{BC,x_k} = 2n$, $k = 1, \ldots, 3$, boundary conditions can be specified independently. To investigate if the boundary conditions are to be specified on the lower or upper bound of the coordinates x_k, $k = 1, \ldots, 3$, the reformulated PDAE system (62)–(67) is transformed into a standard type by algebraic manipulation. To this end, the electric field $\mathbf{E}$ and the concentration of the first species c_1 is eliminated from the model by introducing (66) and (67) into (64) and (65). Further, eliminating the diffusive fluxes by introducing (64) and (65) into the balances (62) and (63) yields

$$\frac{\partial c_k}{\partial t} = D_k \Delta c_k - \frac{z_k F}{RT} D_k \nabla \cdot (c_k \nabla \phi) - \nabla \cdot (\mathbf{v} c_k), \quad k = 2, \ldots, n, \tag{72}$$

$$0 = -\sum_{k=2}^{n} z_k (D_k - D_1) \Delta c_k + \sum_{k=2}^{n} \frac{z_k F}{RT} (z_k (D_k - D_1) + D_k (z_k - z_1)) \nabla \cdot (c_k \nabla \phi). \tag{73}$$

Hence, the reformulated PDAE is reduced to a set of $n-1$ parabolic advection-diffusion PDE (72) and an elliptic PDE (73) showing the structure of Poisson's equation. Thus, the $2n$ boundary conditions that can be specified independently for each coordinate are to be distributed equally at the lower and upper bounds of the coordinates, e.g., in the form of the surface balance equations

$$\mathbf{n}_l^L \cdot \left[-D_k \nabla c_k + \frac{z_k c_k}{RT} D_k F \nabla \phi + \mathbf{v} c_k \right]_{x_l = x_l^L} - \Phi_{k,l}^U (t, x_l \neq x_j) = 0, \tag{74}$$

$$\mathbf{n}_l^U \cdot \left[-D_k \nabla c_k + \frac{z_k c_k}{RT} D_k F \nabla \phi + \mathbf{v} c_k\right]_{x_l = x_l^U} - \Phi_{k,l}^L(t, x_l \neq x_j) = 0, \tag{75}$$

$k = 2, \ldots, n, \quad j = l = 1, \ldots, 3,$

and the Dirichlet conditions for the electric potential

$$\phi|_{x_l = x_l^L} = \phi_l^L, \tag{76}$$

$$\phi|_{x_l = x_l^L} = \phi_l^U, \quad l = 1, \ldots, 3. \tag{77}$$

Here, $\mathbf{n}_l^L$ and $\mathbf{n}_l^U$ correspond to normal vectors in the direction of x_l pointing into the domain at the lower and upper bounds of x_l. $\Phi_{k,l}^L$ and $\Phi_{k,l}^U$ are known fluxes entering or leaving the domain across the boundaries. The electric potential at the boundaries is prescribed by ϕ_l^L and ϕ_l^U. This specification of $n-2$ surface balance equations and the electric potential difference at each boundary of the system is in good agreement with heuristics derived from physical arguments.

As a final result the modeling work-flow results in the reformulated model (62)–(67) with initial conditions (71) and boundary conditions (74), (75), (76) and (77).

5.2. Incompressible Navier–Stokes equations

The incompressible Navier–Stokes equations for a Newtonian fluid are

$$\frac{\partial \mathbf{v}}{\partial t} = -\mathbf{v} \cdot \nabla \mathbf{v} - \frac{1}{\rho} \nabla p + \frac{\eta}{\rho} \Delta \mathbf{v} + \mathbf{f}, \tag{78}$$

$$0 = \nabla \cdot \mathbf{v}, \tag{79}$$

where $\mathbf{v}$ is the local velocity vector $\mathbf{v} = [u, v, w]^T$, p the pressure, η the constant kinematic viscosity and ρ the constant density of the fluid. The external force $\mathbf{f}$ is considered as a known input for the sake of simplicity.

5.2.1. Index analysis and reduction

Obviously, system (78) and (79) is in semi-explicit form with respect to time, so that no reformulation of the model is required in step 4 of the proposed algorithm. The index analysis with respect to time carried out in step 5 reveals $\nu_{d,t} > 1$, as (79) is an MSSS. The reduction in steps 7–10 reveals the additional constraint

$$g_{add,t} = 0 = -\nabla \cdot (\mathbf{v} \cdot \nabla \mathbf{v}) - \frac{1}{\rho} \Delta p + \nabla \cdot \mathbf{f}, \tag{80}$$

where the identity (79) implies $\nabla \cdot \Delta \mathbf{v} = 0$ is used.

The additional constraint (80) is used to substitute one scalar member of the momentum balance equations (78). The resulting model formulation

$$\frac{\partial u}{\partial t} = -\mathbf{v} \cdot \nabla u - \frac{1}{\rho} \frac{\partial p}{\partial x_1} + \frac{\eta}{\rho} \Delta u + f_{x_1}, \tag{81}$$

$$\frac{\partial v}{\partial t} = -\mathbf{v} \cdot \nabla v - \frac{1}{\rho} \frac{\partial p}{\partial x_2} + \frac{\eta}{\rho} \Delta v + f_{x_2}, \tag{82}$$

$$0 = -\nabla \cdot (\mathbf{v} \cdot \nabla \mathbf{v}) - \frac{1}{\rho} \Delta p + \nabla \cdot \mathbf{f} \tag{83}$$

$$0 = \nabla \cdot \mathbf{v}, \tag{84}$$

is characterized by $\nu_{d,t} = 1$. Thus, the method returns to step 4 to reformulate the model as a pseudo-DAE system which is semi-explicit in the next independent variable x_1. The subsequent index analysis with respect to x_1 yields $\nu_{d,x_1} = 1$, so that the method returns to step 4. The subsequent analysis steps with respect to x_2 and x_3 yield $\nu_{d,x_2} = 1$ and $\nu_{d,x_3} = 1$.

5.2.2. Physical interpretation and consistent initial and boundary conditions

The additional constraint (80) highlights the fact that the dynamics of the system are characterized by only two storage terms, one less than apparent in the original formulation. The additional constraint (80), referred to as Pressure-Poisson equation (David Shirokoff, 2011), is well known in the CFD literature and used for the investigation of the consistency of boundary conditions (Gresho and Sani, 1987), the development of projection methods (Guermond and Quartapelle, 1998) or directly for the numerical solution (David Shirokoff, 2011). It is interesting to note that the proposed procedure can derive this important relation, which is hidden in the model structure without any a priori knowledge.

Despite the improved insight into the system's properties, the reduction procedure provides only very limited information regarding the consistency of initial and boundary conditions. This is due to the fact that the reformulated model (81)–(84) requires – like the structure of the original model – tailored methods for the discretization, e.g., in form of a staggered grid, for the implementation of boundary conditions and for the numerical integration (Kwak and Kiris, 2010; Patankar, 1980) and cannot be solved as a simple evolution problem in time as in the examples presented before. Moreover, the structure of the reformulated model seems to be less suited for numerical treatment, since the symmetry in the spatial coordinates is lost. Still, the reformulated model explicitly displays the differential degrees of freedoms with respect to time and spatial coordinates. Thus, as $d_{f,t} = 2$, two initial conditions can be specified independently, e.g.,

$$u(t = t_0, \mathbf{x}) = u_0(\mathbf{x}), \tag{85}$$

$$v(t = t_0, \mathbf{x}) = v_0(\mathbf{x}). \tag{86}$$

On the hyperplane $t = t_0$, the third velocity component, in this case w, is uniquely determined by Eq. (84). The differential degrees of freedom with respect to x_1 and x_2 are $d_{f,x_1} = 6$ and $d_{f,x_2} = 6$, so that in total $n_{BC,x_k} = 6$, $k = 1, 2$, boundary conditions can be specified independently at the upper or lower bound of the coordinates x_1 and x_2. For x_3 the method reveals $d_{f,x_2} = 7$, so that $n_{BC,x_3} = 7$, boundary conditions can be specified independently. A sound evaluation of the consistency of the boundary conditions is not possible with the proposed procedure.

6. Conclusions

In this paper we present a new procedure for the index analysis reduction for distributed PDAE models. It is based on the generalization of established concepts for index analysis and reduction of DAE systems. For this generalization the PDAE system is considered as a set of pseudo-DAE defined on hyperplanes. This motivates the analysis and, if necessary, the reduction of the indices of the pseudo-DAE with respect to the different independent variables in a sequential procedure. In contrast to recent works (Angermann and Rang, 2007; Rang and Angermann, 2005) focusing on a perturbation index for linear PDAE systems, the concept of a differential index is used as it is applicable without any a priori knowledge on the solution of the PDAE system which is not available in the nonlinear case. Further, our method is tailored to a semi-explicit representation of the pseudo-DAE allowing the development of an efficient procedure for index reduction. The latter is based on a symbolic manipulation of the original model equations and eliminates terms that show invariant behavior with respect to specific independent variables. As a result, a reformulated model is obtained which is characterized by differential indices of one with respect to all independent variables.

The procedure can be embedded in a general modeling work-flow for distributed PDAE models. The reformulated model

constitutes an appropriate basis for the specification of consistent initial and boundary conditions and for investigating the applicability of general MOL-based numerical methods. Even more important, the hidden constraints revealed by index reduction provide important information concerning the physical principles implicitly encoded in the model. As such, the method can contribute to an improved understanding of complex coupled PDAE models prior to any numerical studies.

The suggested procedure is demonstrated during the modeling work flow to derive distributed models for a tubular reactor, diffusive charge transport in electrolyte solutions and incompressible fluid flow. In all cases high-index behavior with respect to time and spatial coordinates is observed. For all PDAE systems, the reduction method is capable of deriving equivalent model formulations which are characterized by differential indices of one. Further, a sound physical interpretation can be obtained for the hidden constraints that become explicit in the reduction process. The true number of differential degrees of freedom are identified, which are in all cases less than the apparent number in the original model formulation. These results of the proposed method support the consistent specification of initial conditions in a comprehensive manner. Valuable information for consistent specification of boundary conditions is obtained, including the maximal number of boundary conditions that can be specified independently for a spatial coordinate, though a comprehensive analysis of the consistency of boundary conditions cannot be achieved with the proposed procedure.

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