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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.

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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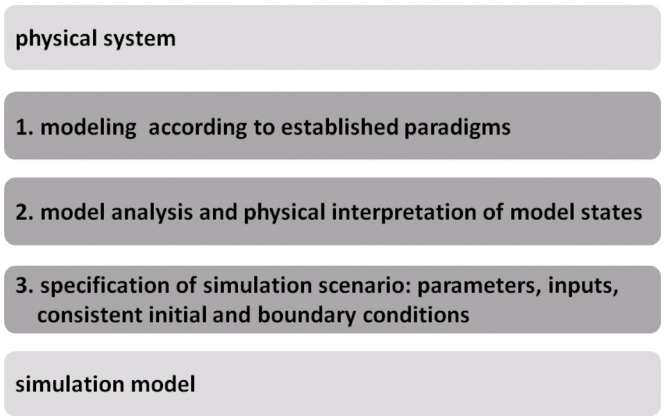

Fig. 1. A general work-flow for the modeling of distributed models.

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