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Converting DAE Models to ODE Models: Application to Reactive Rayleigh Distillation

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This paper illustrates the application of an index reduction method to some differential algebraic equations (DAE) modelling the reactive Rayleigh distillation. After two deflation steps, this DAE is converted to an equivalent first-order explicit ordinary differential equation (ODE). This ODE involves a reduced number of dependent variables, and some evaluations of implicit functions defined, either from the original algebraic constraints, or from the hidden ones. Consistent initial conditions are no longer to be computed; at the opposite of some other index reduction methods, which generate a drift-off effect, the algebraic constraints remain satisfied at any time; and, finally, the computational effort to solve the ODE may be less than the one associated to the original DAE.

1. Introduction

Alloula et al. (2012) introduced the main principles of an original index reduction method by deflation for tackling linear or quasi-linear DAE systems. Part 2 reminds briefly the key features of this method, and of the calculation system implementing it. Part 3 details how a symbolic pre-processing converts a DAE, modelling a reactive Rayleigh distillation, into an ODE model. In this final ODE, implicit functions may appear. Consequently, the main interests are the facts that the equivalent ODE can be integrated numerically by means of the usual ODE solvers, and that the consistent initial value problem is replaced by some implicit function evaluations at the initial time. The main drawback of this nested approach may be the complexity due to the implicit function evaluations. The case study in part 4 gives some feedback after applying the solving framework to a dynamic model of the MTBE synthesis. It appears that, provided that each implicit function evaluation takes advantage of the previous ones, the complexity of integrating the final ODE remains less than the complexity of integrating the original DAE.

2. Index reduction method by deflation

As indicated in Brenan (1996), “multistep and Runge-Kutta methods are not stable and convergent for all higher index DAE systems”. Consequently, those models are usually integrated after applying an index reduction method. But index reduction methods may also have some drawbacks. Apart from the projector-based reductions (Riaza, 2008), or the Kronecker geometric resolutions (Kunkel and Mehrman, 2006, for the linear constant coefficient systems; d’Alfonso, 2011, for quasi-regular systems), the usual index reduction methods consist in differentiating the algebraic constraints, and then solving the resulting differentiated system. However, because the original constraints have been dropped, and replaced by some of their derivatives, such a process may introduce many additional solutions which no longer satisfy the constraints. Usually, the fact that the reduced system is not equivalent to the initial one, results in a drift-off effect. At the opposite, the index reduction method by deflation preserves a local equivalence

between the original DAE and the final ODE. In the following, we remind briefly the main principles of this method, and explain how it can be applied to chemical engineering DAE models.
When dealing with chemical engineering, in many cases, models consist in a set of balances, equilibriums and definitions, which may be written as a first order quasi-linear differential algebraic system:

$$E\big(X(t)\big).\dot{\mathrm{X}}(t) = A(X(t)) \tag{1}$$

where the unknown vector X depends on the dependent variable t.
In the following, we will omit the time dependency for convenience, and will write a first order quasi-linear differential algebraic system as:

$$E(X).\dot{\mathrm{X}} = A(X) \tag{2}$$

E is assumed to be a smooth matrix function with a constant rank on an open subset of $\mathbb{R}^n$. As for E, the nonlinear vector A is assumed sufficiently smooth. Those assumptions mean that the mathematical model does not take into account any discontinuity of some dependent variable. Practically, the application of the index reduction method to a mathematical model implies, at least, that the number of phases in the corresponding physical and chemical system remains constant.
In the case of quasi-linear DAE systems, the index reduction method by deflation mainly consists in finding the hidden algebraic constraints from the non-linearly independent rows of the incident matrix. At each iteration step, the model is replaced locally by a strictly equivalent model, where the number of differential equations is reduced, and the number of algebraic equations is augmented. The equivalent model to be solved is a first-order explicit ODE (3), where f may involve (nested) implicit functions defined by algebraic equations.

$$\dot{\mathrm{Y}} = f(Y) \tag{3}$$

In order to find the equivalent deflated system, symbolic transformation steps are required: matrix decompositions, implicit function derivatives … All those steps, as well as the numerical integration of the deflated system, could be implemented in a symbolic-numeric calculation environment, well suited for handling both symbolic transformation steps and numerical evaluation steps. For this case study, the ODE was obtained by hand from the original DAE. However, it was integrated numerically by means of a legacy symbolic-numeric calculation environment (Alloula et al., 2009), where implicit functions associated to algebraic constraints are:

1. defined and derived symbolically;
2. evaluated numerically at any point, as well as their derivatives.

3. Applying the method to a reactive Rayleigh distillation model

3.1 Original DAE model

The DAE model for reactive Rayleigh distillation depends strongly on the chemical reaction kinetics. Throughout this paper, we consider that no instantaneously equilibrated reaction takes place in the liquid phase. We assume that both phases exist, there is no vapour retention and no chemical reactions in the vapour phase. The vapour phase is considered to be ideal. Heat and pressure policy remain free.
Table 1 gives a list of all the symbols appearing in the fore coming model.

Table 1: Nomenclature

Symbol name	Meaning	Unit
N	Number of components	
R	Number of chemical reactions	
$\tilde{R}$	Number of reactants	
U_l	Liquid retention	mol
V	Vapour flow rate	$mol.s^{-1}$
x_i	Liquid molar fraction of component i	
y_i	Vapour molar fraction of component i	
T	Temperature	K
P	Pressure	

h	Molar liquid enthalpy	$J.mol^{-1}$
H	Molar vapour enthalpy	$J.mol^{-1}$
Q	Heating power	$J.s^{-1}$
K_i	Thermodynamic equilibrium constant for component i	
$\nu_{i,j}$	Stoichiometric coefficient for component i in reaction j	
Qr_j	Heat of reaction j	
a_i	Activity of component i	
Kc_j	Chemical equilibrium constant of reaction j	
k_j	Reaction rate constant of reaction j	
Δ_j	$k_j\left(\prod_{i=1}^{\tilde{R}} {a_i}^{\nu_{i,j}} - \frac{1}{Kc_j}\prod_{i=\tilde{R}+1}^{N} {a_i}^{\nu_{i,j}}\right)$	

According to the previous assumptions, and following the given notations, a mathematical model of reactive Rayleigh distillation may be written as:

$$\begin{cases} \dot{U}_l = \sum_{i=1}^{N}\sum_{j=1}^{R}\left(\nu_{i,j}\Delta_j(T,P,x)\right) - V \\ \forall i \in \{1,\dots,N\}; \dot{\overbrace{x_i \cdot U_l}} = \sum_{j=1}^{R}\left(\nu_{i,j}\Delta_j(T,P,x)\right) - V \cdot y_i \\ \dot{\overbrace{h_l(T,P,x)\cdot U_l}} = Q - V\cdot H(T,P,y) - \sum_{j=1}^{R}\left(Qr_j(T,P)\cdot\Delta_j(T,P,x)\right) \\ \forall i \in \{1,\dots,N\}; y_i = K_i(T,P,x)\cdot x_i \\ \sum_{i=1}^{N} x_i = \sum_{i=1}^{N} y_i \end{cases} \tag{4}$$

This reactive Rayleigh distillation model consists of one global mass balance, N partial mass balances, one energy balance, N thermodynamic equilibriums, and one definition of molar fractions. All the derivatives are derivatives with respect to the independent variable t. Obviously, (4) may be written in the form given in (1), and consequently is a first order quasi linear differential algebraic system. The unknown vector could be defined as $X = (U_l, T, x, y, V)'$, while Q and P remain user-defined variables. One should notice that the number of differential equations, $N+2$, and the number of algebraic equations, $N+1$, does not depend on the number of reactions R.

For such a quasi linear DAE model, the differentiation index is more difficult to define, and to compute, than in the linear case. It is related to the augmented systems, obtained by successive differentiation of the initial DAE (see Brenan, 1996). We proved that, when applying the index reduction method by deflation to any linear time varying DAE, the number of steps equals the differentiation index. We guess that, when applying the index reduction method by deflation to some nonlinear DAE, the number of steps equals the differentiation index too. But this result has not been proved already. Consequently, we guess from the application of the index reduction method, but without calculating the augmented systems, that the differentiation index of (4) is 2.

3.2 Final ODE model

When applying the index reduction method to the original DAE system, some common sub-expressions appear during the calculations. Table 2 gives a list of them, with the symbol names that will stand for them in the final results. Function arguments are omitted to simplify the notations.

Table 2: Abbreviations for common sub-expressions

Symbol name	Definition
$\bar{D}_i$	$1 - K_i - \nabla_{x_i} K \cdot x$
$\bar{\mathcal{K}}_i$	$-\bar{\mathcal{D}}_N^{-1}\bar{\mathcal{D}}_i$
$\bar{\mathcal{H}}_i$	$\frac{\partial h}{\partial x_i} + \frac{\partial h}{\partial x_N}\cdot\bar{\mathcal{K}}_i$
$\bar{\mathcal{L}}$	$\frac{\partial h}{\partial T} + \bar{\mathcal{D}}_N^{-1}\frac{\partial h}{\partial x_N} - \nabla_T K \cdot x$

$\bar{\mathcal{G}}$	$H - h + \sum_{i=1}^{N} \left(\bar{\mathcal{H}}_i + \frac{\bar{\mathcal{L}}\,\bar{\mathcal{D}}_i}{\nabla_T K \cdot x} \right) (1 - K_i)\, x_i$
$\mathcal{M}_i$	$\sum_{j=1}^{R} \nu_{i,j}\ \Delta_j - \left(\sum_{l=1}^{N} \sum_{j=1}^{R} \nu_{l,j}\ \Delta_j \right) x_i$
$\bar{\mathcal{Q}}$	$Q - \sum_{j=1}^{R} Q_{r_j}\ \Delta_j - \left(\sum_{i=1}^{N} \sum_{j=1}^{R} \nu_{i,j}\ \Delta_j \right) h - \sum_{i=1}^{N} \left(\frac{\bar{\mathcal{L}}\,\bar{\mathcal{D}}_i}{\nabla_T K \cdot x} + \bar{\mathcal{H}}_i \right) \mathcal{M}_i$

The index reduction method by deflation applied to (3) provides us the following result. Provided that $U_l \neq 0$, $\partial h/\partial T \neq 0$, $\bar{\mathcal{D}}_N \neq 0$, $\nabla_T K(T,P,x) \cdot x \neq 0$ and $\bar{\mathcal{G}} \neq 0$, there exists $\phi_1 : \mathcal{I} \subset \mathbb{R}^N \to \mathbb{R}$ so that equation (3) is equivalent to the following first order ordinary differential equation system:

$$\begin{pmatrix} \dot{U}_l \\ \dot{x}_1 \\ \vdots \\ \dot{x}_{N-1} \\ \dot{T} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{N} \sum_{j=1}^{R} \nu_{i,j}\ \Delta_j(T,P,x) - \bar{\mathcal{G}}^{-1}(T,P,x,y)\, \bar{\mathcal{Q}}(T,P,x,Q) \\ U_l^{-1} \left(\bar{\mathcal{G}}^{-1}(T,P,x,y)\, \bar{\mathcal{Q}}(T,P,x,Q)\, x_1\, (1 - K_1(T,P,x)) + \mathcal{M}_1(T,P,x) \right) \\ \vdots \\ U_l^{-1} \left(\bar{\mathcal{G}}^{-1}(T,P,x,y)\, \bar{\mathcal{Q}}(T,P,x,Q)\, x_{N-1}\, (1 - K_{N-1}(T,P,x)) + \mathcal{M}_{N-1}(T,P,x) \right) \\ U_l^{-1}\, (\nabla_T K(T,P,x) \cdot x)^{-1} \sum_{i=1}^{N} \left(\bar{\mathcal{G}}^{-1}(T,P,x,y)\, \bar{\mathcal{Q}}(T,P,x,Q)\, (1 - K_i(T,P,x))\, x_i + \mathcal{M}_i(T,P,x) \right) \bar{\mathcal{D}}_i(T,P,x) \end{pmatrix} \quad (5)$$

with

$$\begin{pmatrix} x_N \\ y_1 \\ \vdots \\ y_{N-1} \\ y_N \end{pmatrix} = \begin{pmatrix} \phi_1(T, x_1, \ldots, x_{N-1}) \\ K_1(T,P,x)\, x_1 \\ \vdots \\ K_{N-1}(T,P,x)\, x_{N-1} \\ K_N(T,P,x)\, \phi_1(T, x_1, \ldots, x_{N-1}) \end{pmatrix} \quad (6)$$

and

$$V = \bar{\mathcal{G}}^{-1}(T,P,x,y)\, \bar{\mathcal{Q}}(T,P,x,Q) \quad (7)$$

Equation (6) means that one of the liquid molar fractions, x_N in this case, may be defined as an implicit function ϕ_1 of temperature T, and of the other liquid molar fractions $x_1, \ldots, x_{N-1}$. Of course, in (6), $\phi_1(T, x_1, \ldots, x_{N-1})$ could be replaced by its explicit expression $1 - \sum_{i=1}^{N-1} x_i$. But, from (4) only, the index reduction method could not deduce the definition of liquid molar fractions (8):

$$\sum_{i=1}^{N} x_i\,(t) = 1 \quad (8)$$

More precisely, one can verify that (8) results from (3) and the initial condition $\sum_{i=1}^{N} x_i\,(0) = 1$. Because the proof is based on $\forall k \in \mathbb{N}^\star; \sum_{i=1}^{N} x_i^{(k)}\,(0) = 0$, and not on algebraic elimination only, (8) cannot be viewed as an hidden algebraic equation associated to (4). This fact suggests that, to obtain a more efficient ordinary differential equation, the definition of liquid molar fractions should appear explicitly in the initial differential algebraic system, instead of the global mass balance for example.

Equation (6) means that the vapour flow rate, V, can be computed explicitly at any point (T,P,x,y) from:

- the evaluations of the functions defined in tables 1 and 2;
- the evaluations of the derivatives with respect to T and x of some of these functions.

The number of steps of the index reduction method by deflation gives an upper bound for the differentiation index: 2. But, we do not have to check that this upper bound is reached. The index reduction method exhibits an index 0 system, locally equivalent to the initial DAE.

The ordinary differential equation (4) consists in $N+1$ equations, relating $N+1$ dependent variables $U_l, x_1, \ldots, x_{N-1}, T$. At any time, the remaining $N+2$ dependent variables $x_N, y_1, \ldots, y_N, V$ may be computed by using (6) and (7).

3.3 Numerical integration of the ODE model

First of all, the consistent initial condition problem associated to the original DAE is out of concern with its equivalent first-order explicit ODE. To start the numerical integration, one has only to give initial values to $U_l, x_1, \ldots, x_{N-1}$ and T, the dependent variables of the initial DAE which are also the unknowns of the final ODE. From them, the values of the other dependent variables of the initial DAE are computed, either explicitly or implicitly.

Hairer et al. (2010) give an exhaustive review of the numerical methods for solving non-stiff ordinary differential equations. Hairer and Wanner (2002) extend this review to stiff ordinary differential equations. Depending on the stiffness of the ODE provided by the index reduction method by deflation, one can apply either an implicit Runge-Kutta schema, or a multistep method like a BDF (backward difference formulas) method.

The complexity of any numerical method applied to a first-order explicit ODE (3) can be estimated to be the product of the complexity of each f evaluation, times the number of operations (multiplications) appearing in the integration schema. The number of operations associated to the final ODE integration schema is lower than the number of operations appearing in the original DAE integration schema, mainly because the number of equations has been reduced (deflated) by the index reduction method. Unfortunately, this benefit may be counterbalanced by the fact that the complexity of each f evaluation in (3) may be high when f is defined from (nested) implicit functions.

4. Case study

Previous parts introduced quite a general framework for solving a reactive Rayleigh distillation model. This case study illustrates its application to a reactive ternary system.

4.1 MTBE synthesis

We consider the reaction between iso-butene and methanol to produce methyl tert-butyl ether (MTBE). The thermodynamic data have been extracted from Chen et al. (2002), as well as the rate model. In order to obtain ternary diagrams, instead of three-dimensional diagrams, we omitted the thermodynamic influence of the inert component, n-butane.

We assume the following enthalpy reference: ideal gas, 1 atm, 25°C. With such an assumption, the heats of reaction can be set to zero in (4), (5) and (7).

4.2 Software framework

Durand et al. (2012) provide an up-to-date state-of-the-art of the different methods and tools for chemical process dynamic simulation. For such a domain, they emphasize the interest of a mixed-language approach, ”exploiting the potentiality of numerical libraries in other programming environments and software while preserving their performances”. For this case study, we took advantage of a legacy calculation system (Alloula et al., 2009), where symbolic transformations steps are handled within a computer-algebra context, while numerical evaluations steps are subcontracted to a commercial numerical library (IMSL Fortran Numerical Library 6.0). Usual computer-algebra features, such as formal derivation or formal integration, contribute to the accuracy of the ODE integration. More original features, such as common sub expression sharing or, especially in this case, implicit function efficient evaluation, counterbalance the overhead usually associated to symbolic computations.

4.3 Results and discussion

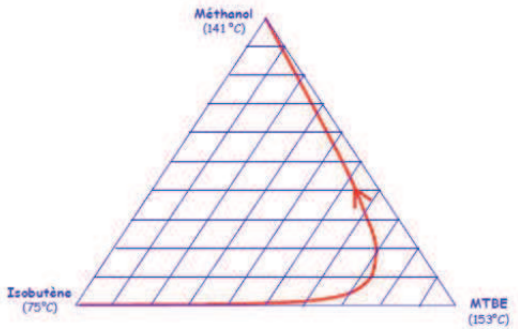

Figure 1: A residue curve for the ternary mixture methanol, iso-butene, MTBE (P=11atm) obtained after integrating ODE (5), assuming $(x_{MTBE}, y_{iso-butene}, y_{methanol}, y_{MTBE})$ *is defined as an implicit function of* $(T, x_{iso-butene}, x_{methanol})$ *(6).*

The main result of this case study is a ternary diagram, which has been compared with the solution obtained by integrating the original DAE. Both diagrams match very closely.
The CPU time required for integrating the final ODE is also very similar to the one required for integrating the original DAE. A simulation taking into account a large number of components and reactions would be more significant, and would give a better insight into the complexity of the index reduction method by deflation. But the first performance results are very promising.
The stability of the equivalent ODE, compared with the initial DAE, has not been studied.

5. Conclusion

The application of an index reduction method by deflation to a DAE, modelling the reactive Rayleigh distillation, provides an equivalent first-order explicit ODE, where implicit function evaluations may appear. This equivalence between the original DAE and the final ODE is the main benefit obtained from the method. Consistent initial conditions are no longer to be computed. At the opposite of some other index reduction methods, which generate a drift-off effect, the algebraic constraints remain satisfied at any time. The case study suggests that the computational effort to solve the final ODE may be less than the one associated to the original DAE, provided that the implicit function evaluations are cached. This way, as time goes on, the overhead associated to implicit function evaluations vanishes.
This symbolic transformation process has been applied to a system where chemical reactions are controlled by kinetics. In the near future, we plan to apply it to a system where instantaneously equilibrated chemical reactions take place. The numerical characteristics of the system to be solved may change. The final goal is to extend such a transformation process to a DAE modelling a reactive distillation column. Because handling by hand the symbolic transformation of the DAE model to an ODE model is a tedious and error-prone process, we are on the way to automate it

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