16th European Symposium on Computer Aided Process Engineering
and 9th International Symposium on Process Systems Engineering
W. Marquardt, C. Pantelides (Editors)

Stability Analysis of Differential-Algebraic Equations in AUTO_DAE

Bianca C. von Clausbruch, Evaristo C. Biscaia, Jr., Príamo A. Melo[a]

[a]*Programa de Engenharia Química/COPPE, Universidade Federal do Rio de Janeiro, Centro de Tecnologia, Bloco G, Sala G116, Ilha do Fundão, Rio de Janeiro – RJ, CEP 21945-970, Brasil.*

Abstract

A new computational package (AUTO_DAE) to study the stability of index-1 differential-algebraic equations (DAEs) is presented. The characterization of the characteristic values of these systems is also presented and a discussion on the stability theorems for ordinary differential equations is performed for the differential-algebraic case. AUTO_DAE is based on the open source continuation and bifurcation computational package AUTO (Doedel *et al*., 1997), thoroughly used to investigate the behavior of ODEs. Prior to steady-state non linear analysis, AUTO_DAE performs a structural characterization of the DAEs in order to recognize the algebraic equations presented in the model. The characteristic values of the DAE system are evaluated using a standard routine to solve the generalized characteristic value problem. Reliability and robustness of the new code are demonstrated through the analysis of non linear chemical engineering problems.

Keywords: DAE; Stability; Continuation; Bifurcation; Software.

1. Introduction

When a process is investigated, model based steady-state and dynamic analysis is usually performed before control and optimization techniques are implemented. Many process models may present non linear responses such as multiplicity of stationary solutions and self-sustained periodic oscillations. In order to study those modes of responses appropriately, one may use the well-known concepts underlying the bifurcation theory as well as methods of parametric continuation.

The theory of nonlinear dynamical systems described by ordinary differential equations (ODEs) is very well developed and there are an uncountable number of academic and scientific books, articles and computational packages about this subject. Nevertheless, the theory for systems governed by differential algebraic equations (DAEs) is not so well developed and is modestly discussed in the open literature, and the main results available are usually obtained for simple cases, such as those described by index-1 DAE systems. Besides, open and public domain computational codes for nonlinear analysis of DAEs are almost nonexistent in the literature (see, for instance, Hyanek *et al*., 1995; Kienle, *et al*., 1995; Ochs *et al*., 1996; Mangold *et al*., 2000).

In this work, a new, open source computational package to study the stability behavior of process models described by index-1 differential-algebraic equations is presented. The new code, AUTO_DAE, is based on the well-known bifurcation and continuation package AUTO (Doedel *et al*., 1997). Prior to steady-state nonlinear analysis, AUTO_DAE performs a structural characterization of the DAEs in order to recognize the algebraic equations presented in the model. The characteristic values of the DAE system are evaluated using a standard routine to solve the generalized characteristic value problem. Reliability and robustness of the new code are demonstrated through the analysis of nonlinear chemical engineering problems.

2. Review of Theory

2.1. Stability of DAEs

The problem of stability and bifurcation analysis of DAE systems has also received attention in other communities than the chemical engineering community (e.g. Reich, 1995; Beardmore and Song, 1998; Chen and Aihara, 2001). A tutorial discussion regarding this subject is presented by Beardmore and Song (1998). When approaching the problem, a few fundamental questions may be posed: *Can the methods of nonlinear analysis developed for ODEs be directly applied to DAEs? Is it possible to define the Lyapunov stability for DAEs? If the DAE system has a given parameter, λ, can one find the bifurcation structure of the solutions as λ is varied?* Unfortunately, preliminary answers to these questions are generally negative.

Nevertheless, if certain *regularization conditions*, given by Reich (1995), are satisfied, it can be shown that the stability of equilibrium points of DAE system can be analyzed using classical linear algebra and spectral theory concepts. Furthermore, in the neighborhood of the equilibrium point, the DAE system possesses a linearization that is a vector field whose flow is equivalent to that of the DAE system, and whose dimension is equal to that of the local manifold (Beardmore and Song, 1998). These results are particularly important when one is interested in applying classical ODEs theory in the study of DAEs and shows, additionally, that a linearization is possible.

The determination of the stability for a DAE system is performed slightly different from the purely differential case. Consider the semi-explicit DAE system below

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \mathbf{f}(\mathbf{x}(t),\mathbf{y}(t),\lambda) \\ \mathbf{0} &= \mathbf{g}(\mathbf{x}(t),\mathbf{y}(t),\lambda) \end{aligned}, \tag{1}$$

where $\mathbf{f}\in\Re^n$, $\mathbf{g}\in\Re^m$ are nonlinear functions, and $\mathbf{x}\in\Re^n$, $\mathbf{y}\in\Re^m$ are differential and algebraic state variables, respectively. The notation may be simplified even more as follows

$$\mathbf{B}\frac{d\tilde{\mathbf{x}}}{dt} = \mathbf{F}(\tilde{\mathbf{x}}(t),\lambda), \tag{2}$$

where $\mathbf{B}\in\Re^{n+m}\times\Re^{n+m}$ has *rank*($\mathbf{B}$)<n+m, $\mathbf{F}=[\mathbf{f}\quad \mathbf{g}]^T\in\Re^{n+m}$, and $\tilde{\mathbf{x}}=[\mathbf{x}\quad \mathbf{y}]^T\in\Re^{n+m}$.

Let $\tilde{\mathbf{x}}^*$ be an equilibrium point of Equation (2). Then, performing a linearization of the system around of the equilibrium point and neglecting high order terms, one may write

$$\mathbf{B}\frac{d(\tilde{\mathbf{x}}-\tilde{\mathbf{x}}^*)}{dt} = \mathbf{A}(\tilde{\mathbf{x}}(t)-\tilde{\mathbf{x}}^*). \tag{3}$$

The matrix $\mathbf{A}\in\Re^{n+m}\times\Re^{n+m}$ is the well-known Jacobian matrix of the system. Thus, the determination of the stability of equilibrium points of Equation (3) gives rise to a generalized characteristic value problem, as follows

$$\mathbf{A}\mathbf{v} = \mathbf{B}\mu\mathbf{v}, \tag{4}$$

where μ is a characteristic value associated to the characteristic vector $\mathbf{v}$. The concept of a matrix pencil may be useful at this point.

Definition (Matrix pencil). Let $\mathbf{A}$ and $\mathbf{B}$ be a pair of matrices n×n. The set of all matrices of the form $\mathbf{A}-\mu\mathbf{B}$, with $\mu\in C$, is called matrix pencil (C is the set of complex numbers). The characteristic values of the matrix pencil are elements of the set $\mu(\mathbf{A},\mathbf{B})$ defined by

$$\mu(\mathbf{A},\mathbf{B}) = \{\mu \in C / \det(\mathbf{A} - \mu\mathbf{B}) = 0\}.$$

If $\mu \in \mu(\mathbf{A},\mathbf{B})$ and $\mathbf{Av} = \mu\mathbf{Bv}$, with $\mathbf{v} \neq \mathbf{0}$, then $\mathbf{v}$ is called characteristic vector of $\mathbf{A}$-$\mu\mathbf{B}$.

As discussed by Beardmore and Song (1998), considering that the DAE system satisfies the regularization conditions given by Reich (1995), which guarantees the existence of the linearization, then it may be said that if all pairs $(\mu,\mathbf{v}) \in C \times C^{n+m}$ satisfying

$$(\mathbf{A} - \mu\mathbf{B})\mathbf{v} = \mathbf{0}, \quad (5)$$

are such that $\mathrm{Re}(\mu)<0$, then $\tilde{\mathbf{x}}^*$ is *linearly stable*. For vector fields linear stability implies in local asymptotic stability (Seydel, 1994), which is also valid for regular DAE systems.

The calculation of saddle-node bifurcation points, also known as limit points, may be carried out using the limit points theorems for ODEs, as they are also equilibrium points of Equation (2). It should be pointed out, though, that the stability of the equilibrium point should be determined as indicated by Equation (4).

As far as Hopf bifurcation points are concerned, Reich (1995) presents a version of the Hopf theorem applied to DAE systems, where the regularization conditions assure the linearization of the system. Reich uses the regularization conditions to justify the Hopf theorems for index-1 DAE systems (Beardmore and Song, 1998).

2.2. Parametric Continuation of Index-1 DAEs

AUTO (Doedel *et al*., 1997) is a continuation package able perform bifurcation analysis of algebraic systems of the form

$$\mathbf{f}(\mathbf{x},\lambda) = \mathbf{0}, \quad (6)$$

where $\mathbf{f} \in \Re^n$ is a vector of nonlinear functions, $\mathbf{x} \in \Re^n$ is a vector of state variables and $\lambda \in \Re$ is a real parameter of the system. Systems of ODEs of the form

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}(t),\lambda), \quad (7)$$

may also be investigated in AUTO.

In order to carry out the continuation of stationary curves, AUTO uses a pseudo-arc length with multiple step predictor-corrector technique (Kubiček and Marek, 1996), as long as the user supplies the code with an initial steady-state, and chooses one or more continuation parameters of the mathematical model. It is possible, then, to detect the occurrence of special points, such as limit points (LP) and Hopf bifurcation (HB) points. Besides, continuation of periodic orbits is also possible, as well as the continuation of LPs and HBs in two or three parameters. A strong limitation of AUTO is that, in principle, DAE systems may not be treated directly. Furthermore, AUTO is designed to work with low dimensional problems. Is should be pointed out, though, that literature shows that AUTO may be easily enhanced to work with systems up to a few hundred equations (Hyanek *et al*., 1995; Melo *et al*., 2003). Besides, linear algebra methods of sparse matrices are available in the literature, as discussed by Mangold *et al*., 2000.

3. Stability Analysis in AUTO_DAE

In order to perform the continuation of stationary points of DAEs in AUTO, the calculation of characteristic values must be performed as indicated by Equation (4). Notice that, at steady-state, Equation (2) reduces to Equation (6), indicating that the continuation algorithm does not require any change. For the solution of the generalized characteristic value problem, the routine `rgg.f` of Eispack (Netlib, 2004) was chosen. This routine uses the QZ algorithm of Moler and Stewart (1973). This algorithm does

not make any inversion of matrix **B** or of any submatrix of **B**, and is a generalization of the QR algorithm (Golub and van Loan, 1996).
It is important to notice that a fundamental step toward the determination of the stability of equilibrium points of a DAE system is the calculation of matrix **B**. In order to do that, a structural characterization routine has been added to AUTO. The vector of functions **F** (cf. Equation (2)) is implemented in AUTO with the aid of another vector, **XPRIME**, as follows

$$\begin{aligned} F_i &= RHS_i - XPRIME_i \quad \text{for } i = 1,...,n \\ F_i &= RHS_i \quad \text{for } i = n+1,...,n+m \end{aligned}, \tag{8}$$

where RHS stands for the right hand side of the equation. Notice that, as presented in Equation (8), the system possesses n differential equations and m algebraic equations. The structural characterization routine tests the existence of derivatives of the state variables in the equations and characterizes the structure of the DAE system. As a result, matrix **B** is generated.
The major modifications of AUTO described above have resulted in a new code for the analysis of steady-state stability of index-1 DAE system called AUTO_DAE. In order to show the reliability and robustness of the new code, two chemical engineering systems that may be described by DAEs are treated below.

4. Examples

4.1. The CSTR with A→B Reaction

The first example is the well-know CSTR with an exothermic first order reaction, A → B, described by Uppal, Ray and Poore (1974). This is a benchmark example for many nonlinear studies as it presents a multitude of nonlinear responses, including multiplicity of steady-state solutions and limit cycle behavior. Mass and energy balances performed on the reactor lead to the following dimensionless mathematical model

$$\frac{dx_1}{dt} = -x_1 + Da(1-x_1)\exp(x_2), \tag{9}$$

$$\frac{dx_2}{dt} = -x_2 + BDa(1-x_1)\exp(x_2) - \beta x_2, \tag{10}$$

where x_1 is the conversion of species A, x_2 is the dimensionless reactor temperature, Da is the Damköhler number, B is the adiabatic temperature rise, and β is the dimensionless heat transfer coefficient.
As presented, the model is described by ODEs and, thus, may be directly implemented in AUTO. In order to test the new version of the code, AUTO_DAE, the model was rewritten in such a way to force the appearance of a differential-algebraic structure. In the index-1 formulation of the model one may write

$$\frac{dx_1}{dt} = -x_1 + Da(1-x_1)x_3, \tag{11}$$

$$\frac{dx_2}{dt} = -x_2 + BDa(1-x_1)x_3 - \beta x_2, \tag{12}$$

$$0 = x_3 - \exp(x_2). \tag{13}$$

Figure 1 presents a typical bifurcation diagram for this system as the Damköhler number is varied. Other parameters were kept constant during the calculation (B=14 and β=2). Saddle-node (limit point) as well as Hopf bifurcations are observed. Stable branches are given by solid lines and unstable branches by dotted lines; Hopf

bifurcation points are represented by the symbol (■). Three bifurcation diagrams were built: two for the implementation of Equations (9)-(10) in AUTO and in AUTO_DAE, and another for the implementation of Equations (11)-(13) in AUTO_DAE. In all three cases, the bifurcation diagrams are rigorously identical to that presented in Figure 1.

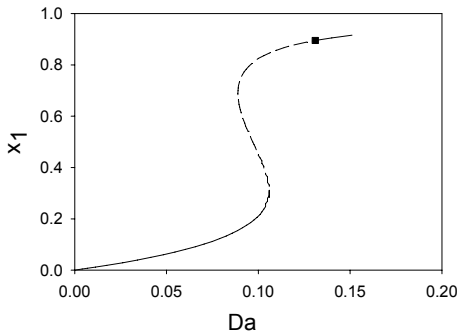

Figure 1 – Bifurcation diagram for Example 1.

4.2. The Evaporative Cooling Reactor

The second example presented regards the evaporative cooling CSTR, also known as *boiling liquid reactor*. In this class of reactors, the reaction heat for exothermic reactions is removed by partial vaporization of the liquid phase (Figure 2a). A first order, exothermic reaction A $\rightarrow$ B is processed in the vessel. By assuming the quasi-steady state hypothesis for the dynamics of the cooling jacket, the reactor mathematical model is given below as presented by Zavala (1997)

$$\frac{dx_1}{dt} = I - O_l, \tag{14}$$

$$\frac{dx_2}{dt} = I - O_l \frac{x_2}{x_1} - kx_2, \tag{15}$$

$$\frac{dx_3}{dt} = \frac{1}{x_1 Cp_l}\{ICp_\ell (x_I - x_3) - \Delta h_r k x_1 + O_g [Cp_l (x_{cond} - x_3) - \Delta h_{vap}], \tag{16}$$

$$O_l = \beta\sqrt{x_1}, \tag{17}$$

$$O_g = \alpha\sqrt{P_0 - P_{cond}}, \tag{18}$$

where x_1 and x_2 represent the total number of mols and the number of mols of species A in the liquid phase, respectively, x_3 is the reactor temperature, O_l is the exit molar flowrate, and O_g is the gas phase molar flowrate (Figura 2a).

For this system, there was no need to create auxiliary algebraic variables, as Equations (17)-(18) guarantee the index-1 differential-algebraic structure for the system. It should be noticed, however, that if Equations (17)-(18) were inserted into Equations (14)-(16), then the system would become purely differential.

All parameters of the evaporative cooling reactor used for the calculations presented here may be found in Zavala (1997), and are omitted here due to space reasoning. In order to test the new code, three bifurcation diagrams were built: two for the implementation of Equations (14)-(16) in AUTO and in AUTO_DAE, and another for the implementation of Equations (14)-(18) in AUTO_DAE. In all three cases, the bifurcation diagrams are rigorously identical to that presented in Figure 2b. A discontinuity in the state equation used for the calculation of vapor pressure of species A is responsible for the unusual behavior observed in Figure 2b.

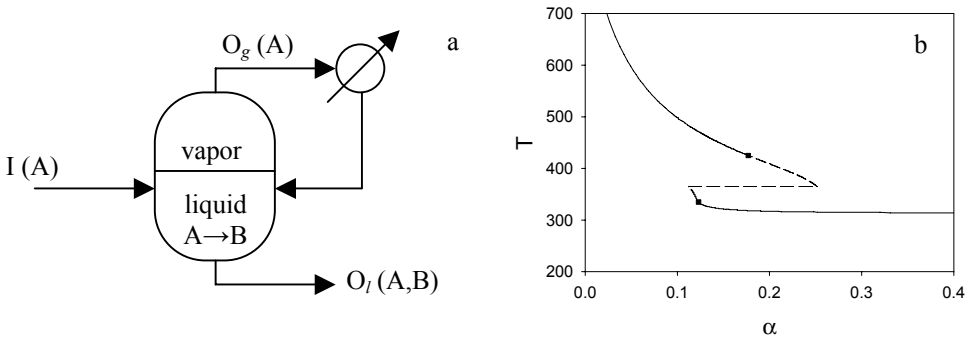

Figure 2 – Sketch (a) and bifurcation diagram (b) of the evaporative cooling reactor.

4. Conclusions

A new code, AUTO_DAE, is presented to perform stability analysis of process models described by differential-algebraic equations. Tests with chemical engineering problems have demonstrated the reliability and robustness of the new code.

5. Acknowledgments

Authors would like to thank CNPQ (*Conselho Nacional de Desenvolvimento Científico e Tecnológico – Brasil*) for providing scholarship to B.C.C. and supporting this research. Comments from ESCAPE reviewers are also acknowledged.

References

Chen, L.; Aihara, K., Stability and bifurcation analysis of differential-difference-algebraic equations. *IEEE Trans. Circ. Syst. I. v. 48(3), p. 308-326, 2001.*

Beardmore, R. E.; Song, Y. H., Differential-algebraic equations: a tutorial review. *Int. J. Bif. Chaos. v. 8(7), p. 1399-1411, 1998.*

Doedel, E.; Champneys, A. R.; Fairgrieve, T. F.; Kuznetsov, Y. A.; Sandstede, B.; Wang, X. *AUTO 97: User's Guide*, Concordia University, Montreal, 1997.

Golub, G.H.; van Loan, C.F. Matrix Computations. London: The Johns Hopkins University Press, 1996.

Hyanek, I.; Zacca, J. J.; Teymour, F.; Ray W. H. Dynamics and stability of polymerization process flow sheets. *Ind. Chem. Res. v.34(11), p.3872-3877, 1995.*

Kienle, A.; Lauschke, G.; Gehrke, V.; Gilles, E.D. On the dynamics of the circulation loop reactor – numerical methods and analysis. *Chem. Eng. Sci., v.50(15), p. 2361-2375, 1995.*

Kubiček, M.; Marek, M. Computational Methods in Bifurcation Theory and Dissipative Structures, New York: Springer-Verlag, 1986.

Mangold, M.; Kienle, A.; Gilles, E.D.; Mohl, K.D. Nonlinear computation in DIVA - methods and applications. *Chem. Eng. Sci., v. 55(2), p. 441-454, 2000* .

Melo, P. A.; Biscaia Jr., E. C.; Pinto, J.C. *The bifurcation behavior of continuous free-radical solution loop polymerization reactors.* Chem. Eng. Sci., *v. 58(13), p. 2805-2821, 2003.*

Moler, C.B.; Stewart, G.W., An algorithm for generalized matrix eigenvalue problems. *SIAM J. Numer. Anal., v.10(2), p. 241-256, 1973.*

Netlib. Netlib Repository. URL: http://www.netlib.org, last accessed in 03/15/2004.

Ochs, S.; Rosendorf, P.; Hyanek, I.; Zhang, X.M.; Ray, W. H. Dynamic flowsheet modeling of polymerization processes using POLYRED. *Comp. and Chem. Eng., v. 20(6-7), p. 657-663, 1996.*

Reich, S. On the local qualitative behavior of DAEs. *Circ. Syst. Sig. Proc., v. 14(4), p. 427-443, 1994.*

Seydel, R. Practical bifurcation and stability analysis – from equilibrium to chaos. New York: Springer-Verlag, 1994.

Uppal A.; Ray W.H.; Poore, A. B. On the dynamic behavior of continuous stirred tank reactors. *Chem. Eng. Sci., v. 29(4), p. 967-985, 1974.*

Zavala, M.S. Some issues in the dynamic modeling and simulation of large-scale systems in chemical engineering. M.Sc. Thesis, University of Wisconsin at Madison, Madison, Wisconsin, USA, 1997.