THE MATHEMATICAL MODELLING OF TRANSIENT SYSTEMS

USING DIFFERENTIAL–ALGEBRAIC EQUATIONS

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ABSTRACT

The mathematical difficulties associated with a class of mixed systems of differential and algebraic equations are presented and an algorithm for dealing with them is described. Two classes of chemical engineering models which give rise to such systems, are identified. Also some problems arising from rigorous dynamic distillation models are analysed.

SCOPE

The mathematical modelling of chemical engineering operations under transient conditions leads naturally to mixed systems of differential and algebraic equations (DAE's).

DAE systems can be classified according to their index. DAE's of index one behave quite similarly to sets of ordinary differential equations (ODE's), and can be solved using similar solution methods. However, the behaviour of DAE's of index exceeding unity is qualitatively different to that of ODE's, presenting special difficulties. In particular, consistent initial conditions for such systems must satisfy not only the original equations themselves, but also the first or higher-order differentials with respect to time of some of these equations. As a result, the number of variables for which arbitrary initial values may be specified is less than the number of differential equations in the system. An efficient graph-theoretical algorithm for detecting the equations, the differentials of which must be taken into account, is presented.

DAE systems of index two or higher arise in chemical engineering models of phase equilibrium processes; they also occur in dynamic "design" problems involving the calculation of a time–varying control necessary for achieving a desired system behaviour.

The index of DAE's describing rigorous dynamic distillation models can be shown to be strongly dependent on the type of pressure specification imposed on the system.

CONCLUSIONS AND SIGNIFICANCE

Dynamic models of some chemical engineering operations give rise to DAE systems, the behaviour of which is qualitatively different to ODE systems. An algorithm for detecting such systems, and overcoming the special problems posed by them, is presented.

1. Introduction

The mathematical models of chemical

engineering systems operating under transient conditions are usually described by mixed sets of differential and algebraic equations (DAE's) of the form:

$$f(x, \dot{x}, y, u, t) = 0 \qquad (1)$$

$$g(x, y, u, t) = 0 \qquad (2)$$

Here $x(t)$ and $y(t)$ are unknown vectors referred to as the "differential" and "algebraic" variables respectively, while $u(t)$ (the "input" variables) are known functions of time, t. Normally, the differential equations (1) arise from dynamic material, energy and momentum balances; processes which are much faster (e.g. thermodynamic equilibrium) yield algebraic equations of type (2), and so do equations defining auxiliary quantities etc.

Many DAE systems are very similar to systems of ordinary differential equations (ODE's). In fact, if the algebraic equations (2) are solvable for the algebraic variables, y given values of the differential variables, x, then the DAE system may be converted to the ODE

$$f(x, \dot{x}, y^*, u, t) = 0 \qquad (3)$$

where $y^* = y^*(x, u, t)$ is the solution of (2). If, furthermore, equations (3) are solvable in $\dot{x}$, they can be rearranged to the standard ODE form

$$\dot{x} = \bar{f}(x, y^*, u, t) \qquad (4)$$

Of course the above transformations may not be a practical method of solution. This is especially true if (2) or (3) are nonlinear in y or $\dot{x}$, in which case sets of nonlinear equations may have to be solved numerically every time the ODE integrator requires the value of the right hand side of (4). However, Gear (1971) showed that such an approach is quite unnecessary, and that DAE's can be solved by an extension of his well-known backward-difference formula (BDF) class of methods, originally developed for ODE's. Briefly, at the kth integration step, Gear's method uses the BDF formulae relating $\dot{x}^{(k)}$ to eliminate $\dot{x}^{(k)}$ from equations (1), thus leaving an essentially algebraic system in $x^{(k)}$ and $y^{(k)}$. The latter is solved using a modified Newton's iteration. Similar ideas can be applied using any implicit or semi-implicit integration formula. Gear's ideas have already formed the basis of successful DAE codes (Petzold (1982b), Morison (1984)).

However, not all DAE systems are similar to ODE's (Petzold (1982a)). For many well-posed problems equations (1) and (2) are not solvable

for variables $\dot{x}$ and y for fixed x. This is exhibited as the singularity of the Jacobian matrix

$$\begin{bmatrix} f_{\dot{x}} & f_y \\ 0 & g_y \end{bmatrix}$$

for all values of x. Not only does this imply that the reduction of the DAE system (1) and (2) to the ODE's (4) through algebraic transformations is not possible, but it also has serious consequences regarding the provision of correct initial conditions for such systems. Furthermore, even if the initialisation problems are surmounted, controlling the truncation error during integration may be problematic.

Section 2 of this paper demonstrates the problems associated with obtaining consistent initial conditions for DAE systmes. The index classification of such systems is introduced, and a recently developed algorithm for consistent initialisation is presented.

Section 3 of the paper shows how DAE systems of the type presented in section 2 arise in chemical engineering applications. Finally, section 4 analyses the special problems presented by rigorous dynamic models of distillation operations.

2. The Initialisation of DAE Systems

For a given DAE system, a consistent initial condition is a set of vectors $\{x(0), y(0), \dot{x}(0)\}$ which must satisfy the constituent equations (1) and (2). Although this requirement is sufficient for many systems, there are some DAE's for which further requirements on the set of consistent initial conditions are imposed by the differentials of some of the equations with respect to time. This is best illustrated in terms of a simple mathematical example.

Consider the linear DAE system

$$\dot{x}_1 = x_1 + x_2 + y \qquad (5)$$

$$\dot{x}_2 = x_1 - x_2 - y \qquad (6)$$

$$0 = x_1 + 2x_2 - y \qquad (7)$$

This can be reduced to an ODE system in x_1 and x_2 by using (7) to eliminate y. Involving the consistency requirement, one can view (5)-(7) as a set of three equations in the five unknowns $x_1(0)$, $x_2(0)$, $y(0)$, $\dot{x}_1(0)$, $\dot{x}_2(0)$; thus two (=5-3) variables may be given arbitrary initial values, and the values of the other three then determined by solving the equations. It should be noted that the number of arbitrarily specifiable conditions equals the number of differential equations in the system, as is always the case with ODE systems.

Consider, however, the DAE system

$$\dot{x}_1 = x_1 + x_2 + y \qquad (5)$$

$$\dot{x}_2 = x_1 - x_2 - y \qquad (6)$$

$$0 = x_1 + 2x_2 \qquad (8)$$

Several difficulties are immediately apparent. First, reduction to ODE's through algebraic transformations is not possible, since (8) cannot be solved for the algebraic variable, y. Furthermore arbitrary values for $x_1(0)$ and

$x_2(0)$ cannot be specified, since the two are now related through (8). In fact, the differential of (8) with respect to time,

$$0 = \dot{x}_1 + 2\dot{x}_2 \qquad (9)$$

must also be satisfied by any consistent initial condition. Thus equations (5), (6), (8) and (9) form a set of four independent equations in the five unknowns $x_1(0)$, $x_2(0)$, $y(0)$, $\dot{x}_1(0)$, $\dot{x}_2(0)$. Consequently, only one of these variables may be specified arbitrarily despite the fact that there are still two differential equations in the system! Of course, having obtained a consistent initial condition, in principle either (8) or (9) need be retained for the actual solution process, but not both since one implies the other. However, numerical considerations involving the control of the truncation error during integration imply that the differentiated form (9) is preferable to (8) (Gear and Petzold (1984)).

Despite their apparent similarity, systems (5), (6), (7) and (5), (6), (8) are qualitatively different, as shown by the above argument. A convenient classification of DAE systems is provided by their index. Here we define index as the minimum number of differentiations with respect to time that the system equations have to undergo to convert the system into a set of ODE's. Thus, by definition any ODE system has index zero. System (5), (6), (8) is of index two: one differentiation leads to (9), or, equivalently, using (5) and (6) to eliminate $\dot{x}_1$ and $\dot{x}_2$, to

$$0 = 3x_1 - x_2 - y \qquad (10)$$

A second differentiation applied to (10) yields an expression for $\dot{y}$,

$$\dot{y} = 3\dot{x}_1 - \dot{x}_2 = 2x_1 + 4x_2 + 4y \qquad (11)$$

which, together with (5) and (6), forms a set of ODE's in x_1, x_2 and y. Similarly, it is easy to show that (5), (6), (7) is an index one system: an expression for $\dot{y}$ may be obtained by a single differentiation of equation (7).

While the initialisation of most index one problems is very similar to that of ODE's, some index-one and all index-two or higher index problems exhibit the type of difficulties exemplified by (5), (6), (8), notably the need to take the differentials of some of the equations into account. It should be noted that not all equation differentials are relevant: for instance, differentiating equation (5) yields

$$\ddot{x}_1 = \dot{x}_1 + \dot{x}_2 + \dot{y} \qquad (12)$$

In principle, equation (12) must be satisfied by the solution of system (5), (6), (8) at all times, including the initial time t=0. However, (12) does not impose any actual constraint on the set of valid initial conditions, since it can always be made true by appropriate selection of the newly introduced variables $\ddot{x}_1$ and $\dot{y}$.

Pantelides (1986) addressed the problem of locating all equations which must be differentiated for the purposes of consistent initialisation, without performing any unnecessary differentiations. In the case of the general system (1), (2), it can be shown that a

variables, i.e.

$$w(t) = \psi(x, \dot{x}, y) \qquad (20)$$

although in most practical cases $w(t)$ are just a subset of $\{x, \dot{x}, y\}$.

Dynamic design problems invariably lead to higher index DAE's if the form of (20) is such that it constrains the differential variables, x to the extent of destroying their independence.

Consider, for instance, a dynamic model of a well-stirred reactor in which a first-order, exothermic chemical reaction takes place. The describing equations are:

$$\frac{dc}{dt} = K_1(c_o - c) - R \qquad (21)$$

$$\frac{dT}{dt} = K_1(T_o - T) + K_2 \cdot R - K_3(T - T_c) \qquad (22)$$

$$0 = R - K_3 \exp(-K_4/T) \cdot c \qquad (23)$$

where:

   c, T are the reactant concentration and
      temperature in the reactor;
   c_o, T_o are the reactant concentration and
      temperature in the feed;
   R is the rate of reaction per unit volume;
   T_c is the coolant temperature;
and K_1, K_2, K_3, K_4 are given constants.

For given feed conditions $c_o(t)$ and $T_o(t)$, the specification of coolant temperature variation, $T_c(t)$ yields a system of three equations in the three unknowns $c(t)$, $T(t)$ and $R(t)$. Since all inputs are given, this is a simulation problem, the solution of which is completely straightforward. In fact, one differentiation of equation (23) yields an expression for dR/dt thus converting the system to a set of ODE's; its index is, therefore, one.

However, if $T_c(t)$ is unknown and one wishes to determine it so that a given desired variation $w(t)$ of the exit concentration, c is achieved, i.e.

$$0 = c - w(t) \qquad (24)$$

one is confronted by a high index problem with all the associated initialisation difficulties. Clearly the differential variable c is not independent, and equation (24) must be differentiated to yield the additional information,

$$0 = \frac{dc}{dt} - \dot{w}(t) \qquad (25)$$

However, further restrictions on the initial conditions can be obtained by differentiating the three equations (21), (23) and (25), since they contain only two distinct members of $\{dc/dt, dT/dt, R, T_c\}$. Again, this introduces three new equations but only two new variables, namely d^2c/dt^2 and dR/dt. These new equations together with (21) − (25) form a set of eight equations in the eight unknowns $c(0)$, $T(0)$, $R(0)$, $T_c(0)$, $dc/dt(0)$, $dT/dt(0)$, $dR/dt(0)$, and $dc/dt(0)$. Thus no variable may be given an arbitrary initial value, despite the fact that the original system (21) − (24) contains two differential equations.

The index of the dynamic design problem (21) − (24) can be shown to be three, whereas that of the associated simulation problem (21) − (23) is

only one. The two are, therefore, qualitatively different. This situation is in sharp contrast to the steady-state case, for which simulation and design problems are mathematically very similar. The latter fact is exploited by the latest generation of steady-state simulators which employ equation-oriented ideas (Perkins (1983)) and allow the user almost unlimited freedom in specifying and solving design and simulation problems. If similar flexibility is to be provided by dynamic simulators, automatic algorithms for dealing with high index problems, such as those described in this paper, must be devised and implemented.

4. Dynamic Distillation Models

A further, dramatic demonstration of the dependence of the index of a DAE system on the specifications imposed on a problem, is provided by rigorous dynamic distillation models.

Assuming perfect homogeneity of the liquid and vapour phases, thermodynamic equilibrium and negligible vapour holdup, the DAE system describing stage i of a distillation column consists of the following equations:

$$\frac{dM_i}{dt} = L_{i-1} + V_{i+1} - L_i - V_i + F_i \qquad (26)$$

$$\frac{d}{dt}(M_i x_{ij}) = L_{i-1}x_{i-1,j} + V_{i+1}y_{i+1,j} - L_i x_{ij}$$
$$-V_i y_{ij} + F_i z_{ij}, \quad j = 1 .. N^c \qquad (27)$$

$$\frac{d}{dt}(M_i h_i) = L_{i-1}h_{i-1} + V_{i+1}H_{i+1} - L_i h_i$$
$$- V_i H_i + Q_i + F_i h_i^F \qquad (28)$$

$$y_{ij}/x_{ij} = K_{ij}(T_i, P_i, \underline{x}_i, \underline{y}_i) \qquad (29)$$

$$\sum_{j=1}^{N^c} y_{ij} = 1 \qquad (30)$$

$$L_i = \Phi(M_i) \qquad (31)$$

$$P_{i+1} - P_i = \psi(M_i, V_{i+1}) \qquad (32)$$

$$h_i = h_{liq}(T_i, P_i, \underline{x}_i) \qquad (33)$$

$$H_i = H_{vap}(T_i, P_i, \underline{y}_i) \qquad (34)$$

where

M_i is the molar liquid holdup on stage i;

L_i, V_i are the molar liquid and vapour flowrates leaving stage i;

F_i is the feed flowrate to stage i;

x_{ij}, y_{ij}, z_{ij} are the mole fractions of component j in the liquid, vapour and feed at stage i;

h_i, H_i, h_i^F are the molar enthalpies of liquid, vapour and feed at stage i;

K_{ij} is the K-value of component j at

subset of the equations must be differentiated if and only if the group of corresponding rows of the matrix

$$A = \begin{bmatrix} f_{\dot{x}} & f_y \\ 0 & g_y \end{bmatrix} \qquad (13)$$

is such that

    (i)   the rows within the group are linearly dependent,

and

    (ii) the rows within any proper subset of this group are linearly independent.

An immediate consequence of these criteria is that systems for which matrix A is nonsingular do not exhibit any special initialisation problems.

Since a system of N equations contains 2^N-1 nonempty groups of rows, examining all of these for the above property is not practical for any but the smallest N. Furthermore, given the numerical rounding errors associated with linear algebra operations, such a process is not even reliable. In order to overcome these problems, Pantelides proposed a graph-theoretical algorithm which analyses the nonzero structure of matrix A. The algorithm is based on the observation that a group of k rows is linearly dependent if they contain nonzero entries in fewer than k columns. Equivalently, a subset of k equations must be differentiated if it contains fewer than k distinct members of the set of variables $\{\dot{x}, y\}$. Thus, for instance, equation (8) must be differentiated since it forms a subset of 1 equation containing 0 members of $\{\dot{x}_1, \dot{x}_2, y\}$. Locating such subsets may be done quite efficiently using concepts developed for solving the assignment problem on bipartite graphs (see e.g. Duff (1981)).

Of course, as soon as a suitable equation subset is located, it is first differentiated and then replaced by its differential; the algorithm is then applied to this modified system in order to locate further subsets. Termination of this process for all well-posed problems is proved by Pantelides. Overall, the algorithm can be shown to be of low computational complexity, and can therefore be used to analyse large DAE systems. However, it should be noted that, since the algorithm is based on purely structural information, some groups of linearly dependent rows of A may escape detection.

3.   Higher Index DAE Systems in Chemical Engineering

DAE systems of index exceeding unity occur in many areas of chemical engineering modelling. Two such areas are presented in this section through representative examples.

The modelling of dynamic equilibrium processes often results in index two or higher systems. This usually happens because the differential variables introduced by the material and energy balances are not independent, but are related through the phase equilibrium relationships.

Consider, for instance, the dynamic model of a fixed-volume condenser with negligible liquid hold-up. For a single component vapour, the relevant equations are:

$$\frac{dN}{dt} = F - L \qquad (14)$$

$$N.C_p. \frac{dT}{dt} = F.C_p.(T_o-T) + \lambda.L - U.S.(T-T_c) \qquad (15)$$

$$p.V = N.R.T \qquad (16)$$

and

$$p = A.exp(-B/T) \qquad (17)$$

where

N is the number of moles of vapour in the condenser;

T, p are the temperature and pressure in the condenser;

F, T_o are the feed vapour flowrate and temperature (given);

L is the exit liquid flowrate;

V is the condenser volume (fixed);

U, S are the heat transfer coefficient and area (fixed);

T_c is the coolant temperature (given);

C_p, λ are the vapour heat capacity, and enthalpy of condensation, assumed constant;

R, A, B are given constants.

For simplicity the perfect gas equation of state, (16) is used for the vapour, and a simple Antoine-type vapour pressure correlation, (17) is employed. No subcooling of the liquid is allowed.

Equations (14) – (17) form a DAE system in the four variables N(t), T(t), p(t) and L(t). However, the two differential variables are not independent, as is easily shown by eliminating p from (16) and (17). Applying Pantelides (1986) algorithm, one detects that subset (16) and (17) must be differentiated, since the two equations contain only one member of the variable set $\{dN/dt, dT/dt, p, L\}$, namely p. Thus, a consistent initial condition must satisfy equations (14) – (17), and also the differentials,

$$V \frac{dp}{dt} = \frac{dN}{dt}.R.T + N.R. \frac{dT}{dt} \qquad (18)$$

$$\frac{dp}{dt} = \frac{A.B}{T^2} exp(\frac{-B}{T}) . \frac{dT}{dt} \qquad (19)$$

Since (14) – (19) are six equations in the seven variables N(0), T(0), p(0), L(0), dN/dt(0), dT/dt(0) and dp/dt(0), only one arbitrary initial value must be supplied. Note that the differentiation of (16) and (17) was indeed "profitable", in the sense that it yielded two extra equations while introducing only one new variable, dp/dt.

System (14) – (17) can be shown to be an index two DAE problem: by using (14), (15) and (18) to eliminate variables dN/dt, dT/dt and dp/dt from (19), and applying a second differentiation to the resulting algebraic equation, one obtains an expression for dL/dt; this together with (14), (15) and (18) forms a system of four ODE equations in N, T, p and L.

A second category of chemical engineering problems giving rise to high index DAE systems is formed by "dynamic design" problems, so called by analogy to their steady-state counterparts. In such problems one or more input variables u(t) are unknown, and one seeks to determine them so that a given desired variation in one or more output variables, w(t) is achieved. In general, the outputs can be known functions of the system

stage i;

T_i, P_i are the temperature and pressure at stage i;

Q_i is the external heat input to stage i;

N^C is the number of components in the mixture being distilled.

Here equation (26) is a total material balance, while (27) are individual component mass balances; one of the latter could be replaced by the algebraic relation

$$\sum_{j=1}^{N^C} x_{ij} = 1 \qquad (35)$$

but this substitution does not affect the arguments to be presented here. Equation (28) is a total enthalpy balance, with the liquid and vapour enthalpies defined by (33) and (34). Thermodynamic equilibrium is ensured by equations (29) and (30). Equation (31) relates the flow of the liquid leaving the stage to the holdup on the stage (as, for instance, in the case of liquid flowing over a weir). Similarly, (32) expresses the pressure drop between two stages in terms of resistance incurred by the vapour flowing through the holes (or valves) in the tray, and also through the liquid on the tray. In general, the exact form of functions Φ and ψ depends on the type and geometry of the trays used.

First, the case of an isolated equilibrium stage is considered. It is assumed that the input stream flowrates $\{L_{i-1}, V_{i+1}, F_i\}$, compositions $\{x_{i-1}, y_{i+1}, z_i\}$ and enthalpies $\{h_{i-1}, H_{i+1}, h_i^F\}$ are known functions of time, and so is the external heat input, Q_i. Furthermore, one of the two pressures $\{P_i, P_{i+1}\}$ is also specified. Although these specifications lead to a valid DAE system, problems with consistent initialisation do occur, since the differential variables $\{M_i, x_i, h_i\}$ are not independent. If P_i is fixed, then the N^C+2 equations $\{(29), (30), (33)\}$ contain only N^C+1 distinct algebraic variables, namely $\{y_i, T_i\}$. On the other hand, if P_{i+1} is fixed, the corresponding equations and algebraic variables are $\{(29), (30), (32), (33)\}$ and $\{y_i, T_i, P_i\}$ with cardinalities N^C+3 and N^C+2 respectively. In either case, the differentials of the relevant equations must be taken into account during initialisation, reducing the number of arbitrarily specifiable initial values by one. Note that this conclusion is not affected if equation (35) is used to replace one of equations (27); the only difference in this case is that (35) itself must be differentiated together with all the other equations listed above.

The interesting question here is how the problems associated with single equilibrium stages propagate in column sections of N stages. Again it is assumed that all material and enthalpy inputs to the system are completely specified, together with one of the two pressures $\{P_1, P_{N+1}\}$.

If one applies the consistent initialisation algorithm (see section 2) to the system resulting from the specification of P_1, it is shown that it

is sufficient to differentiate equations $\{(29), (30), (33)\}$ in each stage once only. The DAE system has index two.

However, if the bottom pressure P_{N+1} is specified, the algorithm reveals that equations $\{(29), (30), (32), (33)\}$ in stage i must be differentiated i times! Under such a specification, the index of the DAE system is N+1.

In order to comprehend the above results, one must observe that if the differential of equation (32) must be taken into account during initialisation, the value of $V_i(0)$ depends not only on $V_{i+1}(0)$ but also on $dV_{i+1}/dt(0)$. Consequently, the vapour flowrate leaving the top stage, $V_1(0)$, depends on the vapour flowrate entering the bottom stage and its first N time derivatives. It is this dependence that leads to the high index of the system resulting from the specification of P_{N+1}.

Clearly, the number of differentiations required render the specification of pressure P_{N+1} highly undesirable. The specification of the top pressure P_1 is much more practical, since in this case, equations must be differentiated at most once. However, even these differentiations may be avoided if the requirement for "perfect control" of this pressure is relaxed. This can be achieved by providing an extra equation linking P_1 to other variables in the first stage, such as V_1. This relation may reflect a control law, for instance:

$$V_1 - V_{1,ss} = K \cdot (P_1 - P_{1,ss}) \qquad (36)$$

where the subscript "ss" refers to steady-state values. Alternatively, it may be a pressure drop equation, governing the flow of vapour between the top stage and the surroundings (or another unit, such as a total condenser), of the form

$$P_1 - P_0 = f(V_1) \qquad (37)$$

It may be shown that the addition of either (36) or (37) to the stage equations leads to a DAE system of index one. Of course, the proportional control law (36) could be extended to a PI controller; however, it should be emphasised that a PID controller would re-introduce the initialisation difficulties by rendering P_1 a differential variable.

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