DYNAMIC MODEL

Asghar Husain and K.V. Reddy
International Center for Water and Energy Systems, Abu Dhabi, UAE

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Contents

Summary

Dynamic models for the various units of the MSF plant are given. The results of simulation are compared for two versions of the brine heater model. Interstage flow and release and flow of non-condensables are discussed in detail. Simulation results for the overall plant are given for a few disturbances. Control loops and various control schemes for the brine heater are outlined.

1. Literature Review

A dynamic model of a chemical process plant is suitable for solving problems which involve the transient behavior of the plant, such as testing various control strategies, process interactions, trouble shooting, reliability and stability analysis, and start-up and shut-down conditions. The true dynamic behavior of a plant can only be simulated by including the model of its control system as well, which is made up of algorithms of the controllers, sensors, transducers, transmitters, and final control elements.

Two types of dynamic models are possible. The first is an analytical model which is based on physical principles, similar to the steady-state model presented earlier. The difference is that, in addition to other process variables, time is also a variable. Hence, time-bound changes in the equipment holdup have to be accounted for. The lumped parameter dynamic process model thus contains ordinary differential equations (ODEs) and supporting algebraic equations, both being non-linear; the system is known as differential-algebraic equations (DAEs). For the ODEs, the initial conditions are either known by experience or calculated by steady-state simulation.

The other type of dynamic model is based on a black-box approach, in which a model with unknown parameters is selected according to previous experience or through experiments. Its structure can also be derived from the analytical model by linearizing the model equations at a certain operating point. Then, the unknown parameters must be determined experimentally, which is known as parameter identification and can be performed on-line or off-line. Where the formulation of the phenomenological models is difficult and complicated, statistical models are developed for control purposes. However, the superiority of the former in understanding the true process behavior is unquestionable.

Before reviewing the reported work on multistage flashing (MSF) dynamic modeling, it is first necessary to discuss "devices" and "connections", which are conceptually two different types of modeling objects and constitute integral parts of a dynamic model of any chemical process including that of seawater desalination.

1.1. Devices and Connections

A device is any delimitable part of a process at a defined hierarchical level of the process decomposition, such as the brine heater in the MSF process or the wall of a single tube in its tube bundle. On the other hand, the connections as denoted by the term itself are entities of the real process which connect the devices; typical examples are the connecting pipes between devices or solid-fluid phase boundaries in the tube bundle.

The devices and connections occur in an alternating sequence in the process representation. Conceptually, they are distinguished by the roles they play in a real process. A device converts the fluxes of mass, energy, and momentum it receives from its surroundings into a characterizing vector of state variables such as pressure, temperature, concentration, etc. In contrast, a connection transforms a driving force, i.e. a difference in some potential determined by the known states of two adjacent devices, into a flux. Commensurate with this distinction, only devices possess a non-negligible volume and thus a holdup for extensive quantities. Hence, in dynamic modeling only devices and not connections display a holdup. The behavior of the device is usually expressed by differential equations, while that of a connection by a set of algebraic equations mapping forces into fluxes. In addition, coupling information is needed to describe the topology of the structure such as a process flow sheet. Moreover, there are signal transformers motivated by the control system in a chemical process which do not depict the physicochemical information of a device. Instead, they represent the input/output behavior of the device. Prototypes of signal transformers, for example, are a thermocouple or a proportional integral (PI) controller.

Thus, modeling gives rise to a set of DAEs for each particular object in the process. The set of modeling equations for the entire plant can then be aggregated using the connectivity relations between the different objects. Numerical pre-processing is then applied to transform the set of equations into a form suitable for solution, e.g. discretization of partial differential equations (PDEs) by some method of lines. Finally, the degree of freedom and the index of the resulting DAE system have to be examined (Unger and Marquardt 1991). If high index problems occur, proper analysis has to be carried out to reduce the index by alternative modeling and/or choice of design specification (Lefkopolous and Stadtherr 1993; Unger et al. 1995).

The symbolic pre-processing involves partitioning of the equation system, derivation of Jacobian matrix, replacing numerically ill-conditioned expressions by well-behaved approximations, etc. For a state-of-the-art review of several topics as outlined above, see Marquardt (1995).

1.2. DAE System and its Index

In general, a DAE system consists of

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

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

in which $x(t)$ and $y(t)$ are the "differential" and "algebraic" vectors, respectively, of unknown variables, both functions of time t, while $u(t)$, also a function of time, is a vector of known variables. Normally, Eq. (1) arises from dynamic material, energy, and momentum balances. On the other hand, much faster processes like thermodynamic equilibria yield type 2 algebraic equations; all auxiliary equations are also of that type. If, for given values of x, Eq. (2) is solvable for y then the DAE system can be converted into ODE form. However, such transformation is not convenient when Eq. (2) is non-linear and has to be solved numerically in each step of integration.

For Eqs (1) and (2), the consistent initial condition is a set of vectors,

$[x(0), y(0), \dot{x}(0)]$,

which must satisfy both the equations. Although this requirement may be sufficient for many DAE systems, there are some DAEs in which differentials of some of the equations in the system with respect to time enhance the consistency requirement of the set of initial conditions. This is illustrated by the following trivial example from Pantelides et al. (1988).

Example: linear DAE system (A)

$$\dot{x}_1 = x_1 + x_2 + y \qquad (3)$$

$$\dot{x}_2 = x_1 - x_2 - y \qquad (4)$$

$$x_1 + 2x_2 - y = 0 \qquad (5)$$

In the above system, Eq. (5) can be used to eliminate the algebraic variable y from Eqs (3) and (4), thus converting them into ODEs in x_1 and x_2. As such, Eqs (3)-(5) are a set of three equations in five unknowns

$x_1(t), x_2(t), y(t), \dot{x}_1(t)$ and $\dot{x}_2(t)$.

Thus, for initial values at $t = 0$, two can be arbitrarily fixed and the remaining three are obtained by solving the equations. In this system, note that arbitrarily specifiable conditions are equal to the number of differential equations in the system. Consider linear DAE system (B) in which the differential equations are the same as Eqs (3) and (4); however, Eq. (5) is replaced by the following equation:

$$x_1 + 2x_2 = 0 \qquad (6)$$

Note that the DAE system (B) comprising Eqs (3), (4), and (6) cannot be converted into ODEs since it is not possible to eliminate algebraic variable y. Moreover, arbitrary values $x_1(0)$ and $x_2(0)$ cannot be chosen since the two are now related through Eq. (6). In fact, the differential of Eq. (6) with respect to t, i.e.

$$\dot{x}_1 + 2\dot{x}_2 = 0 \qquad (7)$$

must also be satisfied by any consistent set of initial conditions. Hence, Eqs (3), (4), (6), and (7) form a set of four independent equations in five unknowns,

i.e. $x_1(t), x_2(t), y(t), \dot{x}_1(t),$ and $\dot{x}_2(t)$.

So only one of these variables can be arbitrarily fixed despite the fact that as before there are two differential equations in the original set of Eqs (3), (4), and (6). Thus, in spite of their apparent similarity, DAE system (A), comprising of Eqs (3), (4), and (5) and system (B), comprising of (3), (4), and (6) are qualitatively different. This difference in DAE system is expressed by their "index".

The "index" is defined as the minimum number of differentiations with respect to time that should be done to convert the DAE system into a set of ODEs. According to this definition, any ODE system has an index of zero. DAE system (A) has an index of one since a single differentiation of 5 gives ODEs. But DAE system (B) has an index of two. The first differentiation leads to Eq. (7), then using Eqs (3) and (4)

$\dot{x}_1$ and $\dot{x}_2$

are eliminated to give

$$3x_1 - x_2 - y = 0 \tag{8}$$

A second differentiation applied to Eq. (8) yields

$$\dot{y} = 3\dot{x}_1 - \dot{x}_2 \tag{9}$$

In this way, two differentiations convert the DAE system (B) into ODEs (Eqs 3, 4, and 9). The initialization of most index one problems is quite similar to that of the ODEs, but some index one and definitely those with higher index problems face difficulties as demonstrated in the case of DAE system (B). Hence, to reduce the index it becomes necessary in such cases to consider differentiation of some of the equations in the original system, with or without subsequent algebraic manipulations. However, as pointed out by Lefkopolous and Stadtherr (1993), any differentiation of the original system presents several problems including loss of information. It is, therefore, always preferable to deal with a DAE system in its original form having an index of one. An algorithm suggested by the same authors helps to select from among different sets of independent equations and variables in index one problem formulation. If this algorithm fails, alternative equations and modeling assumptions should be considered to find one such desired formulation.

1.3. Dynamic Model Solution

As in the steady-state model, the number of equations in the dynamic simulation should be equal to the number of variables plus the number of inputs in order to obtain a unique solution. Here, the equations include not only the model equations, but also all types of correlations to calculate various properties such as densities, thermal conductivities, parameters like heat transfer coefficients, etc. The inputs include attributes of all the input streams (flow rate, temperature, pressure, specific enthalpy, etc.) and fixed constructional parameters (tube inside and outside diameters, lengths, areas, etc.). The dynamic model is then constituted by an initial value problem for a system of ODEs. At initial time (t = 0) all process variables must be known; the steady-state simulation output is a convenient source of such information.

The main problem in the dynamic simulation of an industrial scale process is the solution of a large system of DAEs. For this, not only efficient numerical methods but order reduction methods are also necessary, but one has to contend with the loss of accuracy associated with the latter.

A system of DAEs can be integrated using a standard initial value integrator such as the Runge-Kutta (RK) method or Gear's method. However, the solution of $y(t)$ requires that the Jacobian matrix of Eq. (2) should not be singular. If the Jacobian is invertible, the index of DAEs is one. Alternatively, Eq. (2) can be differentiated to convert it into an ODE, so that the total system of ODEs is solved by using a standard routine. Consistent initial conditions are to be given for the solution of the resulting ODEs. DAEs with an index of more than one are problematic in providing consistent initial values. In some cases, it is possible to transform a higher index system into one having an index equal to one. The index can also be lowered by replacing ODEs by a set of non-linear algebraic equations. It may also be possible in some other cases to avoid the higher index by a proper choice of design specifications and process modeling (Lefkopolous and Stadtherr 1993).

The solution of dynamic models, as in the case of the steady-state, can be obtained stage by stage or simultaneously. The general purpose dynamic simulators like SPEEDUP (Aspen Tech 1991), DIVA (Holl et al. 1988; Kroner et al. 1990), and QUASILIN (Smith and Morton 1988) use methods for the simultaneous solution of model equations whereas DYNAMIC and FLOWPACK II of ICI solve stage by stage. A knowledge-based, flow sheet-oriented, user interface for DIVA has been discussed by Bar and Zeitz (1990). It is concerned with the structuring of the factual knowledge of the chemical engineering modeling domain.

1.4. MSF Modeling

The first attempt in this direction was by Glueck and Bradshaw (1970), who divided a flash stage into four compartments, with streams and capacitances interacting materially and thermally. However, no simulation results were provided. Moreover, their model is over-specified because of a differential energy balance combining vapor space and distillate in the flash stage.

Delene and Ball (1971) also considered four compartments in a flash stage. For a better representation of the cooling brine holdup inside the tubes, they were divided into two well-mixed tanks. The non-condensables in the vapor were not accounted for. To calculate evaporation rates and interstage flow, plant-specific correlations were used. Ulrich (1977) applied this model in simulating a test plant containing six flash stages and found reasonably good agreement between the measured and simulated results on disturbing the steam temperature and brine recycle rates. But significant deviations were noted for disturbances in the cooling water rate, for which no explanation was given.

Fukuri et al. (1985) and Rimawi et al. (1989) solved the dynamic model for a once-through plant by simultaneous solution. The latter observed the trend of various variables for 15 s.

Husain et al. (1992, 1993, 1994) developed a dynamic model considering the flashing and cooling brine dynamics and later the distillate dynamics. The models were solved using the SPEEDUP flow sheeting package. For the reduction of steam flow rate to the brine heater by 26 per cent, the simulation results were compared with the available plant results for the same reduction in the steam flow, noting good agreement between the two. The open loop response of the top brine temperature (TBT) for a step change in the steam flow rate was compared with the actual plant test data. Both the simulation and the plant test results agreed to a sufficient degree qualitatively; for further improvement a truly distributed parameter model is required. Applying a non-linear multivariable constrained model predictive controller (CMPC) to this model, Maniar and Deshpande (1995) claimed significant improvement in the operation of the MSF process.

In their rigorous dynamic model, Reddy et al. (1995a) converted DAEs into ODEs, to avoid propagation of errors generated while solving non-linear algebraic equations. Such a specific purpose simulation program can be extremely fast, making it suitable as a plant simulator for training purposes.

Since seawater or brine is a solution of electrolytes, Marquardt (1996c) recently attempted steady-state and dynamic models of the MSF process in terms of electrolyte thermodynamics characterized by simultaneous physical and chemical equilibria. Two different types of dynamic models are proposed, namely a white-box thermodynamic model consisting of balance equations for each atomic species and a black-box thermodynamic model in which equations are formulated in terms of apparent component concentrations. The latter was implemented in the SPEEDUP using a steady-state flash routine from Aspen Plus capable of electrolyte calculations.

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Biographical Sketch

Asghar Husain received Master of Science degree in Applied Chemistry from the Osmania University, Hyderabad – India in 1948, Bachelor of Chemical of Engineering from the University of Michigan – U.S.A. in 1950 and Doctor of Science from the University of Indonesia in 1958 on submission of a thesis on batchwise distillation. This work has been abridged in Chemical Engineers Handbook by Perry in 4th to 6th edition, a McGraw Hill publication.

He taught at the Technical Faculty of the University of Indonesia at Bandung (1952 -1959) and at the Delhi Polytechnic, Delhi University (1959 – 1961). Then he joined as the Research Scientist in the Regional Research Laboratory (now known as IICT) in his hometown Hyderabad – India, a constituent of the Council of Scientific and Industrial Research (CSIR – Delhi).

He retired from the CSIR in 1984 with the title of Distinguished Scientist. The he served as the Professor of Chemical Engineering at Al Fatah University, Tripoli – Libya (1984-1988). Since 1991, he is associated with ICWES at Abu Dhabi, U.A.E.

He is the Author/co-Author of books on “Optimization Techniques for Chemical Engineers (Mac Millan publication), Modeling and Simulation of Chemical Plants (John Wiley publication). He also edited a book on Integrated Power and Desalination Plants (EOLSS Publishers, Oxford). He guided four Ph.D. thesis, two in the discipline of Chemical Engineering and two on modeling and simulation.