DYNAMIC MODELLING AND SIMULATION: MODELLING CONCEPTS AND MODEL OVERVIEW

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Keywords : Brine Heater, Modelling Concepts, Vapor Phase, Flashed Brine, Condensate Channel, Brine in Tubes

Contents

Summary

After giving a brief summary of basic modelling principles this article addresses the problem of dynamic MSF plant modelling. A MSF plant is systematically decomposed into its major constituents. Each of those can be represented by a submodel. The submodels are sufficiently general to allow for the construction of models for different variants of MSF plants by appropriate aggregations and parameterization. In this way a very flexible mathematical representation of the MSF plant system is achieved. For each of the submodels a certain mathematical description is presented and compared to MSF models suggested in literature.

The intention of this article is to provide an overview of the MSF plant model and the submodels it is constructed of rather than to discuss the interesting questions related to modelling certain phenomena such as the interstage brine flow or non-equilibrium effects. These issues are addressed in more detail in subsequent articles.

1. Introduction

Recent advances in nonlinear process control and operations have given rise to an increasing demand for rigorous dynamic models of chemical processes.

First principle models may be used for an assessment of plant operability at an early design stage in order to indicate necessary design modifications. Another major application of rigorous process models is the design of both linear and nonlinear process control systems and real-time applications. Control laws built on an adequate nonlinear process model may at least improve control system performance and may even render satisfactory control feasible if highly nonlinear and constrained processes are considered. In particular, with model-predictive control - where the control law is computed from a dynamic optimization problem on a moving time horizon - any type of process model of an arbitrary degree of detail can be taken advantage of in principle. Finally, nonlinear rigorous process models are indispensable for the evaluation of control system performance by means of dynamic simulation.

However, the net benefit of applying model based techniques to process control depends crucially on the complexity and the quality of the model being employed. In general, it is not possible to assess the model quality required by a certain application *a-priori*. Neither can one assess the degree of model complexity or detail allowed for certain real-time applications *a-priori*. Therefore, the modelling process is iterative as indicated by the graphical representation given in Figure 1.

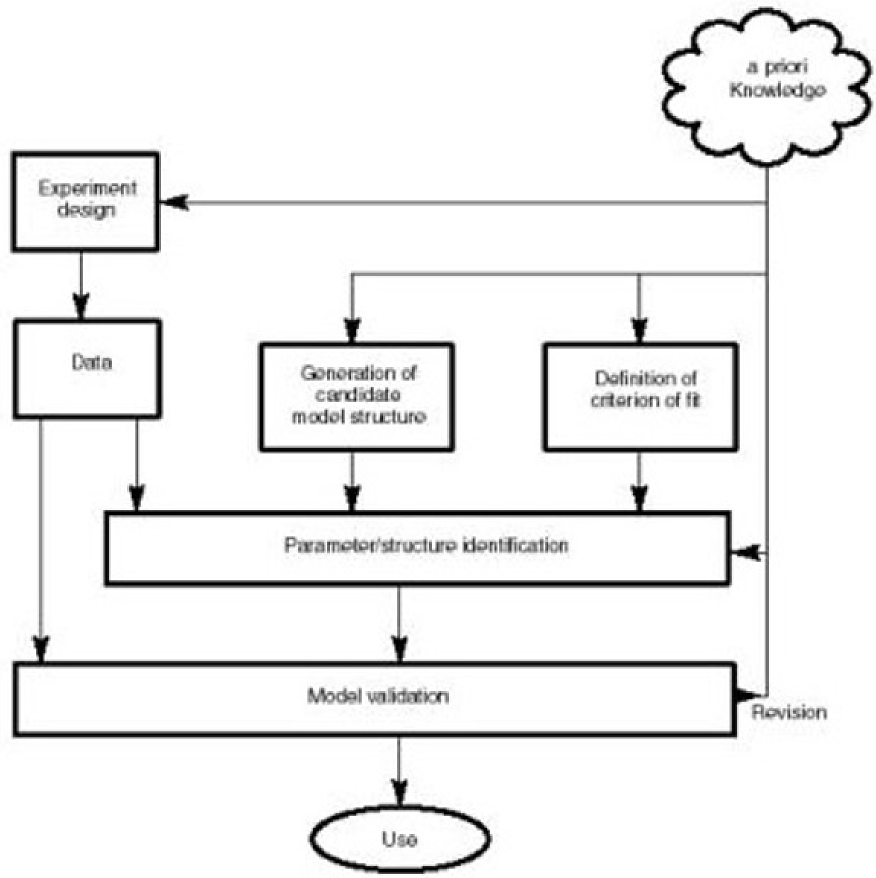

Figure 1. The modelling process.

Various publications address the problem of dynamic MSF plant modelling and simulation (see Bibliography). It would be beyond the scope of this article to give a detailed comparison and assessment of the various model suggestions and the numerical methods employed to solve the system of model equations. However, similarities and differences between the model presented here and those suggested in the literature are discussed. Since most of the literature models are not validated with transient MSF plant measurements it is impossible to give an assessment of their quality. An exception is the results recently reported by Thomas et al. (1998).

A short overview of the basic principles of chemical process modelling is given in section 2. A more thorough treatment can be found in Marquardt (1996). The MSF process is addressed in section 3. The focus here is to give an overview of the generic submodels of which a dynamic model for an entire MSF plant may be constructed, whereas other relevant issues such as modelling of the interstage brine flow, non-equilibrium effects, CO_2 release and brine chemistry or the numerical methods employed to solve the set of model equations are addressed in Chapters - Dynamic modeling and simulation: Brine flow hydraulics; Dynamic modeling and simulation: Non-equilibrium effects and heat transfer. Finally, the suggested MSF plant model is validated in Chapter - Dynamic modeling and simulation: Model validation and simulation studies.

2. Modelling Concepts

According to Marquardt (1996), process modelling may be interpreted as a special kind of general systems development process. In a first step, the process under consideration is decomposed into suitably chosen parts on several hierarchical levels as indicated in Figure 2. Aggregation or decomposition of systems leads to larger or smaller systems. Systems decomposition may extend over several hierarchical levels. It ends on the most detailed level incorporating only elementary systems which are viewed as non-decomposable. These elementary systems and their associated properties determine the granularity (or resolution) of the system description. The choice of hierarchical levels and elementary subsystems is by no means unique but largely oriented by the goals being pursued with the system representation. The chosen granularity given by the set of elementary subsystems is particularly meaningful: a fine granularity increases the need for accurate system knowledge and the effort of developing and using the system representation, whereas a coarse granularity limits its applicability. Similar arguments apply to the choice and type of the hierarchical levels which is driven by the need of varying degrees of abstraction when dealing with complex systems. In all cases a compromise between expressiveness and effectiveness needs to be accomplished.

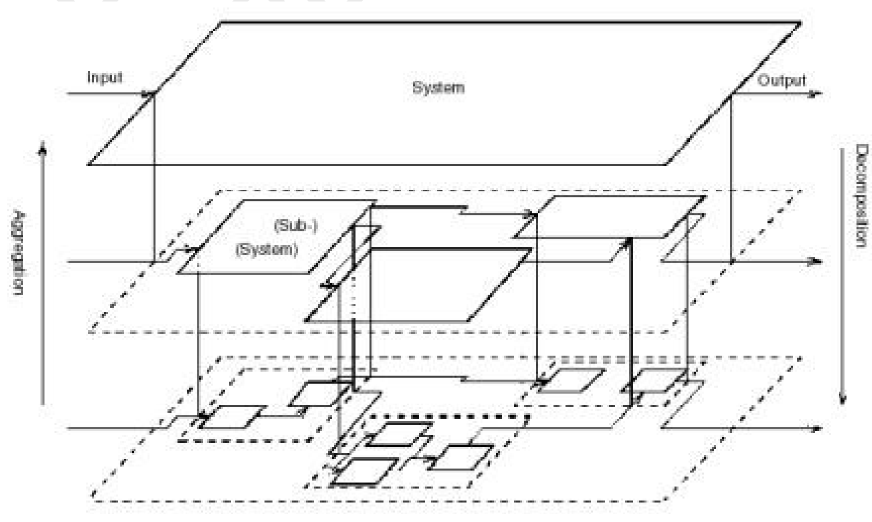

Figure 2. The hierarchical architecture of process systems.

A MSF plant as schematically displayed in Figure 3 may be decomposed on the coarsest level into the heat rejection and the heat recovery section and the brine heater. The heat recovery and rejection sections may be further detailed into the various evaporator stages (see the schematic in Figure 4), each of which is further decomposed into suitable entities as discussed below.

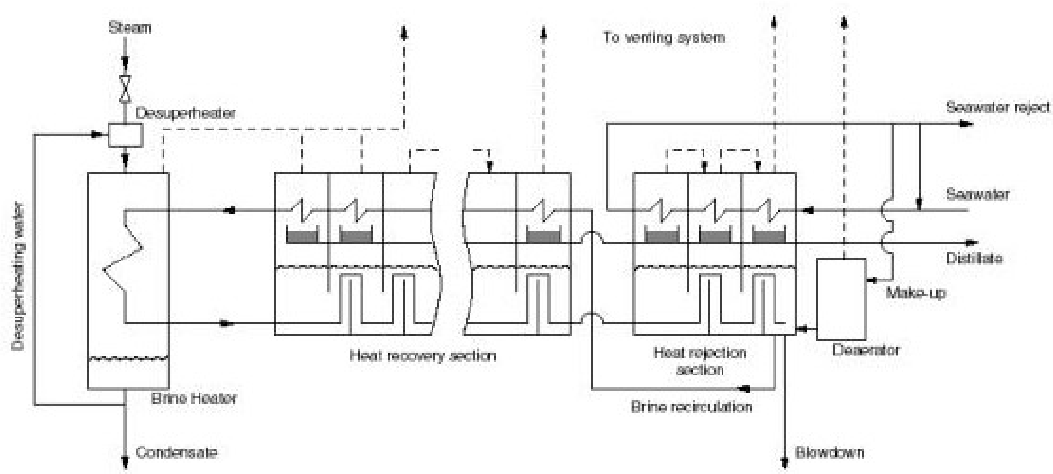

Figure 3. Schematic of brine recycle MSF plant.

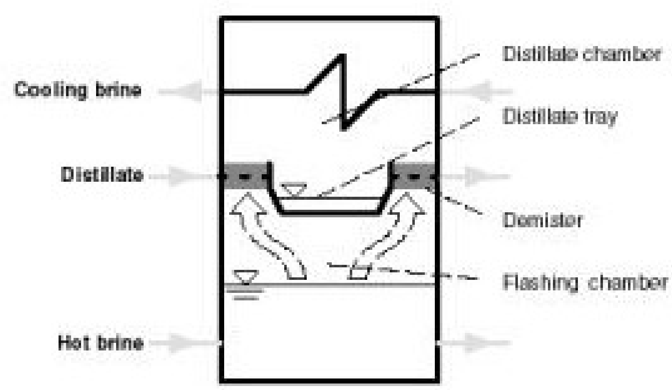

Figure 4. Schematic of an evaporator stage.

Motivated by the structure of a chemical process, two conceptually different classes of modelling objects, namely devices and connections, are distinguished for structure description. Devices represent any delimitable part of a process at a certain level of hierarchical decomposition such as the brine heater or the wall of a single tube in the tube bundle of the heat recovery section. Connections denote all those entities which are situated between devices. Typical examples are the pipes between heat exchangers or the solid-fluid phase boundary between the condensing film and the wall in the tube bundle. Hence, devices and connections occur in an alternating sequence in a process representation. A graphical formalism as shown in Figure 5 is suggested to support process decomposition and abstraction. Devices are shown as labelled rectangular boxes whereas connections are depicted as filled bars associated with arrows pointing to all the devices the connections connects. In some cases a filled bar can also be used as a short cut for a set of connections such as for a graphical representation of all pipes connecting a heat exchanger to the remaining process units. Additional comments to devices or connections may be attached by means of an ellipsoid as depicted in Figure 5. Some principal attributes (for instance the spatial dependency of process quantities) may be included in the graphical representation as indicated by the agitator symbol in Figure 5 characterizing a perfectly mixed phase

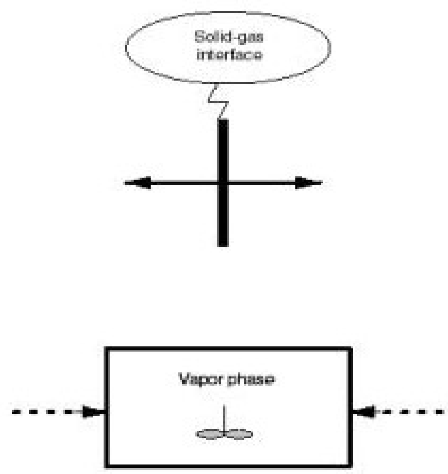

Figure 5. Graphical representation of generic modelling objects: connections (top) and devices (bottom).

The major conceptual distinction between devices and connections is their role in a real process. The role of a device is the determination of some vector of characterizing state variables such as pressure, temperature or concentrations from known fluxes like mass, energy or momentum from the surroundings of the device. Hence, the device responds to flux information by providing state information. In contrast, the role of a connection is the transformation of a driving force (e.g. a difference in some potential) determined by the known states of two adjacent devices into a flux. Complementary to a device, a connection responds to state information with flux information. Consequently, only devices but not connections have a non-negligible volume and hence may display a holdup for extensive quantities. The behavior of a device is usually described by evolutionary equations whereas the behaviour description of a connection is always given by a set of algebraic equations mapping forces into fluxes. Note that connections are subsystems of the process description exactly as devices are. Coupling information (the arrows in Figure 5) is still required to build up a topological structure description on a certain hierarchical level.

Once the structure of a process plant is given in terms of devices, connections and their connectivity relations, each of these elementary modelling objects has to be furnished with a behavioral description comprising two distinct types of concepts: process quantities (the entire set of variables involved in the mathematical process model) and equations. Modelling equations can be characterized as balance equations, constraints and constitutive equations. Balance equations express the change of an extensive quantity (mass, total energy or momentum) in either phases or phase connection. The balances for any other quantity of interest can be derived by refining mass, total energy and momentum by means of constitutive equations and subsequent symbolic manipulation. For instance, it is convenient to derive the energy equation in terms of the measurable process quantities pressure and temperature for a single component system. Constitutive equations have to be added in order to finally determine the equation system of a device or a connection completely. Typical examples of constitutive equations comprise thermodynamic state functions or relations for the calculation of transport coefficients. Constraint equations describe all kinds of algebraic relationships between process quantities which **-** literally or by assumption - have to hold at any time.

The modelling process thus gives rise to a set of partial differential-algebraic equations for each particular modelling object. After completing the behavioral description of every single modelling object, the set of model equations of the entire plant can be derived by means of an aggregation process following the hierarchical structure of the plant and making use of the connectivity relations between the modelling objects. Depending on the numerical methods applied to solve the set of model equations (see Section 8, Dynamic Model), some preprocessing may subsequently be required in order to transform the set of model equations into a form suitable for implementation in a particular simulation tool. A typical example of such a transformation is the discretization of partial differential equations by some suitable method of lines. Finally the degrees of freedom and the index of the resulting aggregated set equations have to be examined, see for example Unger et al. (1995).

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