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Model simplification and time-scale assumptions applied to distillation modelling☆

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ABSTRACT

A generic industrial plant (or section of plant) can be abstracted as a set of capacities exchanging extensive quantities through connecting streams. This abstraction is applicable with different granularities, focusing on smaller or bigger control volumes according on how well the dynamics of the process must be studied. The studied system can be represented as a directed graph, where the capacities are the nodes and the streams are the arcs. The graph of the plant (or of the single operation unit) is a schematisation of the process; the model can then be written as a system of differential and algebraic equations to be solved with a numerical solver. Here we discuss how one can simplify a detailed distillation model. In the studied detailed distillation model, each distillation stage is a dynamic rate-based flash. A cascade of simplified models is accomplished by a systematic procedure that combines singular perturbation and lumping.

1. Introduction

Modelling of industrial processes is today the foundation to almost any operation including design, control, planning and retrofitting. Modelling, model simplification and model reduction are well established areas in process system engineering, and also in control theory. Simplified and reduced models are used both to gain insight into model sub-processes and to ease the computational efforts of simulation and analysis (Taylor, Doyle, & Petzold, 2008). Several model reduction and simplification methods have been developed in the past (Benallou, Seborg, & Mellichamp, 1986; Cho & Joseph, 1983; Khowinij, Henson, Belanger, & Megan, 2005; Kienle, 2000; Kumar & Daoutidis, 2003; Marquardt, 1990, 2001). Among the most popular model simplification techniques, we quote: lumping together similar state variables (Preisig & Westerweele, 2003), projecting a stiff system onto its slow manifold (Maas & Pope, 1992), eliminating states insensitive to parametric perturbation (Turanyi, 1990), and singular and regular perturbation (Robertson & Cameron, 1997).

For a given system or operation, there exist different approaches to develop a dynamic model and its model simplifications; one of these is to use graph theory. Graph theory is an old technique; the first paper about graph theory was published in the 18th century by Leonhard Euler. Despite the old age, graph theory still finds many applications in different disciplines in present problems (Henley & Seader, 1973; Roberts, 1976). In process system engineering, graph theory is used to describe combinatorial and structural aspects of systems (Hangos & Cameron, 2001; Hangos & Tuza, 1999; Jungnickel, 1999; Reinschke, 1988).

Hangos, Szederkényi, and Tuza (2004) propose to study a lumped dynamic process model by bipartite graphs, called equation-variable graphs. In the equation-variable graphs, one class of vertexes represents the set of the equations of the model, while another vertex class contains the modelled variables. This kind of graph is used for analysing the effects of model simplification on the model structure.

In another paper, Hangos and co-workers (Leitold, Hangos, & Tuza, 2002) define the variable structure graph of a dynamic system. This type of graph is a directed graph, where the nodes of the graph are the model's variables (state variables, input variables and output variables), and the directed paths can be used to describe the effect of a variable to the other variables. The variable structure graph finds even earlier applications with Wang's and Cameron's cause-and-effect graphic methods (Wang & Cameron, 1993). In their paper, Wang and Cameron define the cause-and-effect graphs, quoting previous references such as Lin (1974) and Johnston (1990). As the cause-and-effect graph, Lai's and Yu's qualitative model based on signed directed graph (Lai & Yu, 1995) can be considered a reference for the variable structure graph.

The variable structure graph (or simply, the system structure graph) is used to study two common steps of simplifying dynamic

☆ Extended paper of "Graph theory and model simplification. Case study: distillation column" (Dones & Preisig).

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Nomenclature

t	time
$\mathbf{x}$	primary states
$\mathbf{y}$	secondary states
$\mathbf{z}$	transformed primary states
$\hat{a}$	stream of extensive quantity a
$\dot{a}$	time derivative of quantity a
n	mass
U	internal energy
$\hat{\mathbf{n}}_{a\|b}$	mass stream flowing from node a to node b
$\hat{q}_{a\|b}$	heat stream flowing from node a to node b
$\hat{H}_{a\|b}$	enthalpy stream flowing from node a to node b
$\hat{w}_{a\|b}$	volumetric work from node a to node b
A	Helmholtz energy
T	temperature
V	volume
S	entropy
p	pressure
$\boldsymbol{\mu}$	chemical potentials

Subscripts

L	liquid phase
G	gas phase
B	boundary between liquid phase and gas phase

process models, namely the (steady-state) variable removal and the variable lumping simplification (Leitold et al., 2002). These steps are used to simplify those models which display multiple time-scale behaviour. Here, the main operation used to simplify the models is singular perturbation (Martinez & Drozdowicz, 1989; Robertson & Cameron, 1997).

In this context, we propose a model simplification procedure based on graph theory. The starting point is to consider a generic system (*e.g.* a plant or section of plant) as a set of capacities exchanging extensive quantities through connecting streams (Fig. 1). The studied system is modelled with a network approach (Preisig & Westerweele, 2003). Each node of the graph represents a control volume (capacity) connected to the others and to the external of the modelled system by arcs. These arcs are the connecting streams of extensive quantities (Mangold, Motz, & Gilles, 2002; Preisig, 2009b; Westerweele, 2003).

This kind of abstraction is applicable with different levels of detail, focusing on smaller or bigger control volumes according on how well the dynamics of the process must be described (Hildebrandt, Raden, Petzold, Robinson, & Doyle, 2008).

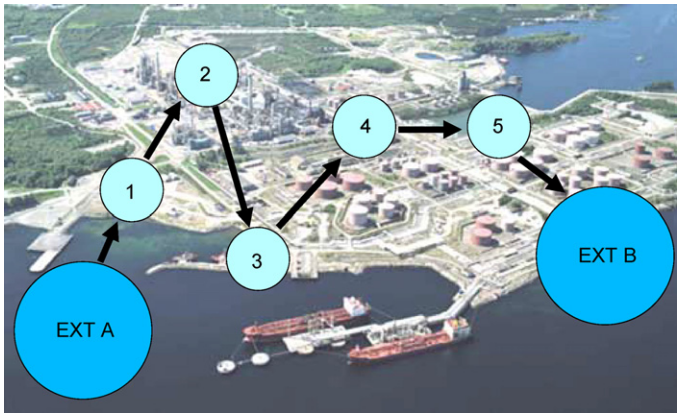

Fig. 1. Graph theory to model industrial plants. The control volumes are uniform lumps (nodes) exchanging extensive quantities (arcs). Picture: StatoilHydro's Mongstad refinery (Norway).

A compact network model of the studied system is as follows:

$$\dot{\mathbf{x}} = \mathbf{F}\hat{\mathbf{x}} \tag{1}$$

Eq. (1) presents a non-reacting system. $\mathbf{x}$ is a stack of vectors of primary states (capacities) of the conserved extensive quantities of the plant (mass, energy and momentum). In (1), the variation in time of the holdups is obtained by summing the streams entering the desired node and subtracting the streams leaving that node. The matrix $\mathbf{F}$ is the stream direction matrix, an incidence matrix made of zeroes, plus and minus ones. The purpose of matrix $\mathbf{F}$ is to map the flows $\hat{\mathbf{x}}$ (mass, energy and momentum streams) and link them to each balance.

Eq. (1) builds the conservation balances for mass, energy and momentum. The arcs of the graph ($\hat{\mathbf{x}}$) are defined in (2) as function of $\mathbf{x}$ and of the related secondary states $\mathbf{y}$, namely chemical potentials, temperatures and pressures.

$$\hat{\mathbf{x}} = \mathbf{g}(\mathbf{x}, \mathbf{y}, t) \tag{2}$$

The intensive variables $\mathbf{y}$ are calculated through transformations of the fundamental state variables $\mathbf{x}$ defined in the conservation equation.

$$0 = \mathbf{h}(\mathbf{x}, \mathbf{y}, t) \tag{3}$$

Eq. (3) defines the state variable transformations. It also contains those variable transformations depending on the thermodynamics and the state equations (Løvfall, 2008).

A formally correct formulation of the plant model is a system of differential and algebraic equations (DAE problem). The dynamic behaviour is studied integrating in time the resulting system (4) (Aascher & Petzold, 1998; Brenan, Campbell, & Petzold, 1996; Buzzi-Ferraris & Manca, 1998; Gear, Leimkuhler, & Gupta, 1985; Manca & Buzzi-Ferraris, 2007).

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{F}\hat{\mathbf{x}} \\ \hat{\mathbf{x}} = \mathbf{g}(\mathbf{x}, \mathbf{y}, t) \\ 0 = \mathbf{h}(\mathbf{x}, \mathbf{y}, t) \end{cases} \tag{4}$$

Defining

$$\mathbf{F}\hat{\mathbf{x}} = \mathbf{F}\mathbf{g}(\mathbf{x}, \mathbf{y}, t) = \mathbf{f}(\mathbf{x}, \mathbf{y}, t) \tag{5}$$

the system in (4) is in the form of a Hessenberg index-1 problem (Campbell & Petzold, 1983; Petzold, 1989; Petzold, 1992):

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{y}, t) \\ 0 = \mathbf{h}(\mathbf{x}, \mathbf{y}, t) \end{cases} \tag{6}$$

In (6), there are explicit differential equations in $\mathbf{x}$ plus algebraic equations (implicit, in the most generic case) clearly separated by the differential equations.

Given a plant/system, a multitude of models may be required, for different purposes or even for the same operation.

The issues related to the modelling task are the difficulty and the time required to generate different models for the same system, and the risks associated to correctly update all of them.

A systematic way to obtain different models with different assumptions is to start with a master model and then to derive a cascade of more simplified models using a simple and precise procedure, which does not leave any room for human error.

Our aim here is to formalise a set of model simplification techniques applicable to mechanistic models. The techniques being discussed here are associated with order-of-magnitude assumptions, singular perturbation and lumping (combination of variable transformation and singular perturbation).