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Structured modeling for processes: A thermodynamical network theory

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Abstract

We review the use of bond graphs for modeling of physico-chemical processes. We recall that bond graphs define a circuit-type language which root on a thermodynamical consistent definition of its network elements. We present the bond graph basic elements in the light of lumped models arising from chemical engineering. We first illustrate it on the historical example of the diffusion process through a membrane. The examples of a Continuous Stirred Tank Reactor and an adsorption process illustrate how the network structure and the choice of variables ease the reusability of submodels and localize the changes in models to some network elements.

Keywords: Thermodynamics; Circuits; Network thermodynamics; Generalized bond graph; Structured modeling

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1. Introduction

Even if mathematical models have been widely accepted as a useful tool for the systematic development of processes, their formulation and their structuring for this purpose remain an active domain of research. Several authors proposed general concepts for the structuring of chemical engineering process models (Bogush, Lohmann, & Marquart, 2001; Gilles, 1998; Hangos & Cameron, 2001; Mangold, Motz, & Gilles, 2002; Marquardt, 1996; Ponton & Gawthrop, 1991; Preisig, 1996). Based on these concepts of representation, different software tools for automating the development of process models have been proposed (Bogush et al., 2001; Mangold et al., 2002; Mattson, Elmqvist, & Otter, 1998; ; Mattsson & Andersson, 1993; Stephanopoulos, Henning, & Leone, 1990; Tränkle, Zeitzand, Ginkel, & Gilles, 2000). They deal with the developments of languages and supporting softwares which allow the storage, reuse, exchange and maintenance of dynamic models in order to enhance the design and optimization of processes and their control.

Some of these structuring concepts are based on the assumption that any dynamical model may be decomposed into primitives that may be assembled in order to compose the total model (Gilles, 1998; Marquardt, 1996). These primitives may be units as well as elementary physical phenomena, depending on the level of the modeling required at the particular stage of design. In this paper we shall deal with the level of storages and phases, according to the terminology given in Gilles (1998), Mangold et al. (2002), that is the level of description of the fluxes of momentum, mass and energy and their coupling (which may be later assembled to form the model of a process unit). At this level, the primitives are thermodynamic properties of a phase and some phenomenological laws. The model is then described in terms of some "blocks" connected by some signals flows, as it is standardly used in automatic control and signal processing. But they differ from block diagrams in the sense that they define classes of variables, such as *currents* or *vectors* in Marquardt (1996) or *potentials* or *current* in Gilles (1998), as well as classes of blocks, such as *component* or *coupling* blocks for Gilles (1998) and *devices* and *connections* for Marquardt (1996) or Preisig (1996) according to the concepts of chemical engineering.

However there exists an alternative graphical tool, called *bond graphs* (Karnopp, Margolis, & Rosenberg, 2000; Paynter, 1961) which is also known under the name of *network thermodynamics* (Oster, Perelson, & Katchalsky, 1973) and which combines a network approach with the axioms of Irreversible

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Nomenclature

$F_{b_e}^{\text{extra}}$	molar inlet flow of constituent b
$F_{b_s}^{\text{extra}}$	molar outlet flow of constituent b
F_e^{extra}	molar inlet flow vector
F_s^{extra}	molar outlet flow vector
k_1, k_2	constant coefficient of the Langmuir's model
K_b^{intra}	mass exchange coefficient between extragranular volume and intragranular one for b
K_b^{ads}	mass exchange coefficient between intragranular volume and the adsorbent for b
n^{extra}	mole number vector in extragranular fluid volume
n_a^{extra}	mole number of a in extragranular fluid volume
n_a^{intra}	mole number of a in intragranular fluid volume
n_b^{extra}	mole number of b in extragranular fluid volume
n_b^{intra}	mole number of b in intragranular fluid volume
n_b^{ads}	mole number of b in the adsorbent
N^{intra}	diffusion flux vector between extragranular and intragranular volume
N_a^{intra}	diffusion flux between the extragranular and the intragranular volume
N_b^{intra}	diffusion flux between the extragranular and the intragranular volume
N^{ads}	diffusion flux vector between the intragranular volume and the adsorbent
N_a^{ads}	diffusion flux between the intragranular volume and the adsorbent
N_b^{ads}	diffusion flux between the intragranular volume and the adsorbent
q_b	molar concentration in b in the adsorbent
P	pressure
P_0	environment pressure
S^{intra}	exchange surface between extragranular and intragranular volumes
S^{ads}	exchange surface between intragranular volume and adsorbant
T	temperature
V^{extra}	extragranular volume
V^{intra}	extragranular volume
y_b^{extra}	mole fraction of component b in extragranular volume
y_b^{intra}	mole fraction of component b in extragranular volume

Greek letters

μ^{extra}	chemical potential vector in extragranular volume
μ_e^{extra}	chemical potential vector at inlet of extragranular volume
μ_a^{extra}	chemical potential of component a in extragranular volume
μ_b^{extra}	chemical potential of component b in extragranular volume
μ^{intra}	chemical potential vector in intragranular volume
μ_a^{intra}	chemical potential of component a in intragranular volume
μ_b^{intra}	chemical potential of component b in intragranular volume
μ_b^{ads}	chemical potential of component b in the adsorbent
μ_b^*	chemical potential of pure component b in fluid at constant T and P

Thermodynamics (Breedveld, 1984b). The main advantage of bond graphs with respect to other methodologies is that

- No assumption is made on computational causality: *currents* are not automatically produced by differences of potential. This potentiality enhances the reuse of models when constraints are changed.
- The pair of signals is power conjugate. That is to say the power is implicitly present in the graph. Since power and energy are general concepts, the bond graph is able to represent any of the physical phenomenon that can be encountered in engineering.

Furthermore bond graphs are supported by a series of softwares such as 20-sim® developed by Controllab products, MS1 by Lorenz Simulation, CAMP-G from Cadsim Engineering (see Borutzky, 2006 for more details) or MTT a free software licensed under the GNU General Public License (MTT, 2004). Finally let us note that languages such Modelica, that are primary a means to exchange models, supports some bond graph libraries.

Bond graphs are widely used in mechatronics (i.e. for controlled electro-mechanical systems). For processes, after the pioneering work of Oster and Perelson (Auslander, Oster, Perelson, & Clifford, 1973; Perelson & Oster, 1975), it has been mainly used for membrane processes (Atlan & Thoma, 1987; Thoma & Atlan, 1990b), some reaction processes (Auslander et al., 1973; Couenne, Jallut, Maschke, Breedveld, & Tayakout, 2006; Oster et al., 1973; Perelson & Oster, 1975; Thoma & Atlan, 1990) and some electrochemical processes (Karnopp et al., 2000). Let us notice that some authors use an alternative way of modelling named "pseudo bond graph" (Heny, Simanca, & Delgado, 2000) for which the pairing of variables are no more power conjugate. Pseudo bond graph can be considered as a graphical tool which follows the usual chemical engineering formulation as presented in Marquardt (1996) or Gilles (1998).

In this paper, we aim to give a chemical engineering oriented introduction to the bond graph modeling language for processes and suggest that it is particularly suited for the modular modeling of processes as its network structure ensures the possibility of writing the equilibrium and continuity equation at the interfaces by the use of conjugated variables as interface variables.

Section 2 of this paper is devoted to the presentation of the bond graph approach. Through two detailed examples described respectively in Sections 3 and 4, we respectively address the representation of heat transport phenomena coupled with mass transport and chemical reactions and of the multi level feature of the process models.