

Basis for bond-graph modeling in chemical engineering

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Abstract

The aim of this paper is to briefly present the Bond Graph language and the advantages that one can get from its use. The main point is the easy reusability of the sub-models that are the basis of a given model. The Bond Graph language has been firstly developed for the modeling of finite dimension systems in mechatronic and electrical engineering but it can also be applied to infinite dimension systems as well as to chemical engineering systems. Such an application is related to the concepts of irreversible thermodynamic.

Keywords: dynamic systems, structured modeling, network, irreversible thermodynamic

1. Introduction

The representation of dynamic models in chemical engineering by using graphs or networks has been already described [1,2]. Such an approach can be very efficient for model management. The model of a system can be manipulated as a set of interconnected and reusable sub-models, provided that softwares are available to support such a manipulation. The Bond Graph language is an example of this kind of tool. It is based on the energetic behavior of the sub-models and their interconnection by using power conjugate variables. It has been mainly applied to finite dimension mechanical and electrical systems [3].

It is supported by commercially available softwares (20-sim® developed by Controllab products, MS1 by Lorenz Simulation, CAMP-G from Cadsim Engineering or MTT, a free software licensed under the GNU General Public License) [4]. Extension of the Bond Graph language to infinite dimension systems has been published [5] as well as applications to chemical engineering problems [6-8]. In this domain, one has to use the entropy as the power conjugate variable associated with the temperature, according to thermodynamic concepts [8,9]. In this paper, we briefly present the Bond Graph language and the way transport phenomena equations can be represented.

2. The Bond Graph language

A Bond Graph is based on multi-port elements related by one- or multi-bonds represented by oriented half arrows. With each bond is associated a set of power conjugate variables, the effort variables e_k and the flow variables f_k . As far as f_k is the flux of the extensive variable q_k , $e_k f_k$ is an energy flux or power associated with the energy form k [3,11]. The **C** capacitive element is associated with the accumulation of the energy H as well as with the accumulation of the extensive variables q_k . The balance equations defining the **C** element as well as a graph example are as follows:

$$H(e_1(q_1, q_2), e_2(q_1, q_2)) :: \overset{f_2}{\downarrow} \underset{e_1}{\leftarrow} \overset{f_1}{\downarrow} \left\{ \begin{array}{l} \frac{dq_k}{dt} = f_k \\ \frac{dH}{dt} = \sum_k e_k(q_j) \frac{dq_k}{dt} = \sum_k e_k(q_j) f_k \end{array} \right. \quad (1)$$

The **0** and **1** junctions represent the transport of the extensive variables as well as of the energy through the graph ($\varepsilon_k = \{1, -1\}$ is a sign convention):

$$\begin{array}{c} f_2 \downarrow e_2 \\ \downarrow f_1 \\ \leftarrow e_3 \quad \mathbf{0} \quad \leftarrow e_1 \end{array} \left\{ \begin{array}{l} \sum_k \varepsilon_k f_k = 0 \\ e_1 = e_2 = \dots = e_k \end{array} \right. \quad \begin{array}{c} f_2 \downarrow e_2 \\ \downarrow f_1 \\ \leftarrow e_3 \quad \mathbf{1} \quad \leftarrow e_1 \end{array} \left\{ \begin{array}{l} \sum_k \varepsilon_k e_k = 0 \\ f_1^k = f_2 = \dots = f_k \\ \sum_k \varepsilon_k e_k f_k = 0 \end{array} \right. \quad (2)$$

The **0** junction represents the continuity of the power and flow variables while the effort variable is common to the bonds. The **1** junction represents a relation between the effort variables and the flow variable is common to the bonds. The resistive element **RS** is dissipative:

$$\frac{\sigma_s}{T} \mathbf{RS} \begin{array}{c} \leftarrow f \\ \leftarrow e \end{array} \left\{ \begin{array}{l} \sigma_s T = \sum e_k f_k \\ \phi(e_j, f_j) = 0 \end{array} \right. \quad (3)$$

It represents the power loss $T\sigma_s$ due to irreversible phenomena where the

power conjugate variables σ_s and T are respectively the total entropy production and the temperature [9]. Relations between efforts and fluxes, that may be coupled, are given by the ϕ function.

Finally we introduce a key element for distributed parameter systems modeling: the multi-port differential transformer element or DTF [5] which is a power preserving structure permitting to express interconnection between the power conjugate variables within the system Ω and at its boundary $\partial\Omega$. This element is the generalization of the transformer element TF [3] and is based on the Stoke's theorem:

$$\begin{array}{c} \overleftarrow{f^2} \\ \overleftarrow{e^2} \end{array} \text{DTF} \begin{array}{c} \overleftarrow{f^1} \\ \overleftarrow{e^1} \end{array} \left\{ \begin{array}{l} f^1 = df^2 \\ e^2 = de^1 \\ \int_{\partial\Omega} e^1 f^2 = \int_{\Omega} f^2 e^2 + \int_{\Omega} f^1 e^1 \end{array} \right. \quad (4)$$

The general notation d stands for the gradient or the divergence according to the nature of the variables that are manipulated.

3. Bond graph representation of transport phenomena

3.1. Energy conjugate variables for the unit of mass of a thermodynamic system

The total energy per mass unit \hat{h} is given by $\hat{h} = \frac{v^2}{2} + u$ that one can differentiate:

$$d\hat{h} = \mathbf{v} \cdot d\mathbf{p} + du = \mathbf{v} \cdot d\mathbf{p} + Tds - Pd\mathbf{v} + \sum_{i=1}^N \mu_i d\omega_i \quad (5)$$

$v = \|\mathbf{v}\|$ is the velocity modulus, u and \mathbf{p} the internal energy and the momentum per mass unit. In equation (5), the conjugate variables associated with the kinetic energy are the velocity and the momentum per mass unit. The Gibbs equation defines the energy conjugate variables for the internal energy [9]. μ_i is the chemical potential of the i component, ω_i its mass fraction, s and \mathbf{v} are the entropy and the volume per mass unit. According to the Bond Graph approach, a balance equation is expressed for the extensive variables associated with the quantities per mass unit $(\mathbf{p}, s, \mathbf{v}, \omega_i)$.

3.2. Balance equations for the extensive variables

These balance equations are written by using the substantial time derivatives defined with respect to \mathbf{v} which turns to be the mass average velocity [10]:

$$\left(\sum_{i=1}^N \rho_i \right) \mathbf{v} = \rho \mathbf{v} = \sum_{i=1}^N \mathbf{f}_i \quad (6)$$

$\mathbf{f}_i = \rho_i \mathbf{v}_i$ is the mass flux of component i , ρ_i its mass concentration and \mathbf{v}_i its velocity with respect to a fixed frame. The extensive variables balances are then as follows:

$$\begin{cases} \rho \frac{Dp}{Dt} = -\nabla \cdot (\phi_p - \rho \mathbf{v} p) + \sum_{i=1}^N \rho_i \mathbf{g}_i = -\nabla \cdot \phi_p^R + \sum_{i=1}^N \rho_i \mathbf{g}_i & (a) \\ \rho \frac{Ds}{Dt} = -\nabla \cdot (\mathbf{f}_s - \rho \mathbf{v} s) + \sigma_s = -\nabla \cdot \mathbf{f}_s^R + \sigma_s & (b) \\ \rho \frac{Dv}{Dt} = \nabla \cdot \mathbf{v} & (c) \\ \rho \frac{D\omega_i}{Dt} = -\nabla \cdot (\mathbf{f}_i - \rho \mathbf{v} \omega_i) + \sigma_i = -\nabla \cdot \mathbf{f}_i^R + \sigma_i \quad i=1..N & (d) \end{cases} \quad (7)$$

$\rho \mathbf{v} p$, $\rho \mathbf{v} \omega_i$ and $\rho \mathbf{v} s$ are the convected fluxes of momentum, component i and entropy. Relative fluxes are then defined with respect to these convected fluxes.

$\phi_p^R = \phi_p - \rho \mathbf{v} p = P \mathbf{I} + \boldsymbol{\tau}$ is the relative momentum flux where P is the pressure and $\boldsymbol{\tau}$ the viscous part of the momentum flux (or shear stress tensor).

$\mathbf{f}_i^R = \mathbf{f}_i - \rho \mathbf{v} \omega_i$ is the diffusion flux and $\mathbf{f}_s^R = \frac{f_q}{T} + \sum_{i=1}^N f_i^R s_i$ is the relative

entropy flux where f_q is the heat flux by conduction and s_i the partial entropy per mass unit. σ_i is a source term for the component i due to chemical reactions. By adding the components mass balances over all the species (equations (7d)), one finds the global space balance (7c) without any source term since it is a conserved quantity. As far as the momentum is also a

conserved quantity, $\sum_{i=1}^N \mathbf{f}_i \cdot \mathbf{g}_i$ is an exchange of momentum with the

surrounding due to the external body force \mathbf{g}_i exerted on the mass unit of component i . According to the second principle of thermodynamic [9], the entropy source term σ_s corresponds to a true creation of entropy:

$$T \sigma_s = -\mathbf{f}_s^R \cdot \nabla T - \sum_{i=1}^N \mathbf{f}_i^R \cdot (\nabla \mu_i - \mathbf{g}_i) - \sum_{i=1}^N \mu_i \sigma_i - \boldsymbol{\tau} : \nabla \mathbf{v} \geq 0 \quad (8)$$

where \cdot is a tensor product [10]. $T\sigma_s$ is a volumetric dissipated power due to irreversible processes that are considered, respectively in the RHS of equation (8), heat transfer, mass transfer, chemical reactions and viscous effects.

3.3. The assumption of local equilibrium

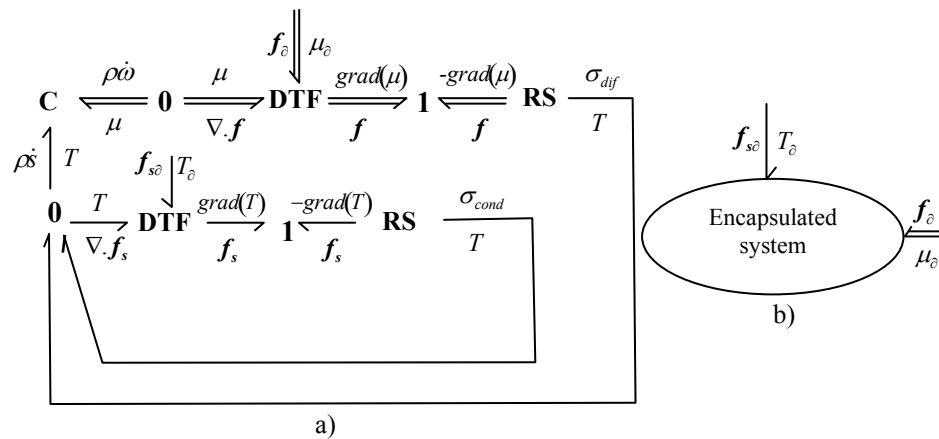
At a sufficiently small scale, equilibrium is reached at each time and the substantial times derivatives $\frac{Dh}{Dt}$, $\frac{Dp}{Dt}$, $\frac{Ds}{Dt}$, $\frac{Dv}{Dt}$ and $\frac{D\omega}{Dt}$ are assumed to satisfy the equation (5) according to the following C element:

$$\begin{array}{c} \dot{s} \downarrow T \\ \overrightarrow{\Psi} \quad \quad \quad \overleftarrow{\dot{\omega}} \\ \mathbf{v} \quad \quad \quad \mu \\ \quad \quad \quad \downarrow -P \\ \overleftarrow{\Psi} \end{array} \quad \rho \frac{Dh}{Dt} = -\nabla \cdot (\mathbf{f}_h - \rho \mathbf{v} \dot{h}) + \sum_{i=1}^N \mathbf{f}_i \cdot \mathbf{g}_i = -\nabla \cdot \mathbf{f}_h^R + \sum_{i=1}^N \mathbf{f}_i \cdot \mathbf{g}_i \quad (9)$$

The energy conservation (9) is deduced from equations (7) and (8) where the flux \mathbf{f}_h can be found in [9,10] and $\sum_{i=1}^N \mathbf{f}_i \cdot \mathbf{g}_i$ is the exchanged energy due to the external body forces.

3.4. Example

Let us consider the Bond Graph represented below.



It is an isochoric system only subject to diffusive heat and mass transfer corresponding to equations (7b) and (7d). These two irreversible phenomena are

represented by two **RS** elements. The fluxes constitutive equations are assumed to be decoupled: the entropy flux f_s is given by the Fourier law while the diffusion fluxes vector f is related to the chemical potential gradients. The bonds connected to the **DTF** elements represent the boundary conditions.

4. Conclusions and perspectives

The above-described Bond Graph a) can be encapsulated in the form b) in such a way that it can be connected to another Bond Graph only through the external ports. Provided that softwares are available, one can easily manipulate and re-use sub-models and connect them through these ports.

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References

1. E. Gilles, Chemical Engineering Technol., 21 (1998) 121
2. M. Mangold, S. Motz and E. D. Gilles, Chemical Engineering Science, 57 (2002) 4099
3. D. Karnopp, D. Margolis and R. Rosenberg, Systems Dynamics a Unified Approach. John Wiley and Sons, New York, 2000
4. <http://www.bondgraphs.com/software.html>
5. A. Baaiu, F. Couenne, D. Eberard, C. Jallut, Y. Legorrec, L. Lefevre, B. Maschke and M. Tayakout-Fayolle, A port-based formulation of transport phenomena, 5th MATHMOD conference, Vienna, Austria, February 8-10, 2006
6. G. F. Oster, A. S. Perelson and A. Katchalsky, Quarterly Reviews in Biophysics 6(I) (1973) 1
7. J. Thoma and B. Bouamama, Modelling and simulation in thermal and chemical engineering, Springer, 2000
8. F. Couenne, C. Jallut, B. Maschke, P. C. Breedveld and M. Tayakout, Mathematical and Computer Modelling of Dynamical Systems, 12(2-3) (2006) 159
9. S. R. De Groot and P. Mazur, Non-equilibrium thermodynamics, Dover, 1984
10. Bird R. B., Stewart W. E., Lightfoot E. N. (2002), Transport phenomena, 2th edition, Wiley
11. P. C. Breedveld, J. of The Franklin Institute, 319 (1985) 136