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Abstract of doctorate thesis

Applications of Bond Graph modelling

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Complex systems modelling rises particular problems and requires theoretical developments based on physics fundamentals. The physical reality model is generally obtained using theoretical concepts considering only the main phenomena that describe the systems. For such situations the control engineers use mathematical models that in spite of their good flexibility loose the physical signification of the system imposing certain limits on further improvements. Due to multidisciplinary nature of physical systems, the communication and data exchange between experts from different fields suffer. Therefore within systems modelling research one main target is a general methodology common to all systems types nondependent on their nature.

An approach that responds to these tasks used to model different nature systems is the Bond Graph methodology. This method is based both on the power transfer between different parts or components of the system and energy transformations within these components (dissipation, storage or conversion of energy field). These phenomena similar to all physics domains are graphic represented and consequently the Bond Graph method represents a common language for modelling of different fields systems.

The main target of the present work is ***the improvement of Bond Graph methodology for modelling of electro-mechanic systems and its development for application in modelling of complex thermochemical and biotechnological processes***. Therefore the study complies with the above mentioned research direction solving problems related to modelling of both physical-technical electrical systems and chemical and biological processes from different application domains in a unified manner.

Industrial processes are strongly non-linear due mainly to high interaction degree of the phenomena. The behaviour of these systems is currently described using non-linear differential equations wising laborious classical methods such as state equations. The Bond Graph model can keep, in this case, the system physical nature enabling the direct location of the state variables within the system.

The study is structured in five chapters undertaking gradually, with respect to developing status of Bond Graph concept at international level, the modelling of electrical, mechanical, electromechanical, thermochemical and biotechnological systems.

First chapter presents the base concepts of Bond Graph method. In order to establish the frame for Bond Graph models development, the fundamentals of constituent elements are presented together with models construction procedures, causality and the causality assignment - one of the methodology major advantages. Based mainly on power transfer between different system parts or components and energy transformations within these components the modelling using this method consists in locating the physical system properties followed by their representation through ideal energy storage, dissipation or transformation elements and the graphical exploitation of the connection between these elements. Using the energy variables a unitary modelling of systems characterized by different energy forms is insured. Considering unique the causal connection between elements, from the Bond Graph model result the linear or non-linear mathematical models as state equations or transfer functions,

information on the system dynamic variation domains and assigned variables and also the model block schema.

In order to highlight the methodology potential an ***analogy between systems of different nature is performed together with the deduction of mathematical models as state space equations using both classical modelling methods and the Bond Graph and also the block diagrams starting from the Bond Graph model.*** The examples proved the unitary specificity of the modelling environment and in good agreement with classical methods.

The **second chapter** is dedicated to Bond Graph structural properties required for the study of different natures systems control laws. First, it is presented a comparison between the structural approach for the general case and the Bond Graph structural approach through structural rank study, together with controllability and observability properties of the state space model.

For a system structural properties analysis, required by the study of control laws, we noticed that is sufficient the representation of links between Bond Graph variables and Bond Graph model parameters independent of their representation – numerical values, symbols or analytic relations.

Another approach in the study of these properties was accomplished starting from the Bond Graph junction structure containing information both on system elements and interconnection mode, independent on their numerical values. Through the study of ***structural properties of different orders linear systems containing different Bond Graph elements*** we highlight that Bond Graph model can be considered an appropriate, fast and easy to use method for the analysis and the study of control laws. The analysis of a dynamic system is necessary at several levels, from control law design to the implementation phase.

The last part of the chapter is dedicated to Bond Graph models structure and inversability property required by the study of input-output decoupling.

Third chapter consists in implementing Bond Graph method in modelling of electric, mechanic and electromechanical systems. The modelling of electric, mechanic systems preceded the electromechanical ones. Therefore the procedures used for these systems modelling lead to a unitary construction methodology for the electromechanical systems. For these systems, mathematic models associated to Bond Graph ones were made and time evolution of main process variables were presented together with the corresponding block diagrams.

The implementation of Bond Graph methodology in physical systems modelling was performed starting with two filters containing R, L, C elements, one eleven order high-pass filter, and one five order low-pass filter, followed by the methodology implementation for mass-spring-damper translation mechanical systems, vertical and horizontal plane oscillating and for rotation mechanical systems.

In the last section dedicated to mechanical systems, an electromechanic equipment was modelled: the direct current motor with permanent magnet, and two rotational Quansers experiments: with flexible arm and inverted pendulum. For these systems the time evolutions of the main process parameters were presented, and block diagrams and mathematical models

associated to the Bond Graph models were obtained significantly easier compared to classical modelling methods.

The distinct approach of different systems types lead to the ***possibility to create modules that can be used in the structure of other Quanser units developed under Bond Graph methodology, highlighting another main characteristic – the modularity***. Consequently, it becomes possible to introduce or to eliminate elements or subassemblies without starting over the whole modelling procedure.

This study conducted to conclusion that electrical and mechanical systems can be easily modelled using Bond Graphs, transposing the technical schemas to simplified models with the condition of good understanding of physical phenomenon that governs the system, the major difficulty in models construction.

In **chapter four** the Bond Graph method is extended, by developing models for chemical reactions based processes and introducing the thermal component of theses processes. A specific approach adapted to physical system particularities – the Pseudo Bond Graph - was used in modelling of thermochemical processes with large industrial scale application. Specific combustion processes were modelled using pure combustible elements and classic multi-component fuels under oxygen and air atmosphere. The approach of the reactions type was performed gradually according to their complexity, starting with single reaction processes and mono-component reactants to processes defined by several reactions with different kinetics and multi-component reactants and several by-products.

The first studied category of processes was high exothermic thermochemical processes. The modelling of these processes was done in an original manner by introducing a supplementary Bond Graph concept compared to previous studied systems – the heat of reaction as function of reaction kinetic, the process energy balance respectively – and using the pseudo Bond Graph. This Bond Graph version uses as effort and flow variables the concentration, the molar / mass flow for chemical stage of the model and temperature, heat flow respectively for thermal stage. Consequently, both Bond Graph model and the dynamic one are structured in two parts connected through ***a multiport modulated resistive element RS that provides information on the reaction kinetic and released heat flow. This element particular to each process type represents an important own contribution in this work***.

The Bond Graph modelling of ***combustion thermochemical processes, an important contribution to the field*** was undertaken gradual with respect to chemical reactions complexity.

Within the first category of reactions the carbon combustion under oxygen atmosphere was modelled and time variations of reactants and products concentration together with process temperatures were simulated. Within modelling of combustion processes with multi-component reactants two reactions using oxygen and air were used. The first reaction, methane combustion, presents the characteristics of theoretical combustion with two reactants and two reaction by-products.

The second reaction was chosen to represent a real combustion process, air representing the common oxidizer at industrial level. The elemental composition of the combustion products together with the process type and reactor characteristics conditioned the mechanisms of by-products formation. Consequently, using an extra amount of air compared to the stoichiometric

one and a fuel composed of six elements, a complex burning process was modelled in order to establish the time evolutions for by-products and reactants concentrations with respect to process temperature. To exemplify, the Bond Graph model (Fig. 1) corresponding to below general combustion reaction is presented:

$$C_zH_yO_xCl_wS_vN_u + r\left(z+\Phi+v-\frac{x}{2}\right)O_2 + r\left(\frac{79}{21}\right)\left(z+\Phi+v-\frac{x}{2}\right)N_2 \xrightarrow{r}$$

$$\xrightarrow{r} zCO_2 + 2\Phi H_2O + wHCl + vSO_2 + \left[\frac{u}{2} + r\left(\frac{79}{21}\right)\left(z+\Phi+v-\frac{x}{2}\right)\right]N_2 + (r-1)\left(z+\Phi+v-\frac{x}{2}\right)O_2$$

where: *z*, *y*, *x*, *w*, *v*, *u* represent the molar fractions of carbon, hydrogen, oxygen, chlorine, sulphur and nitrogen in one mol of fuel; *r* represents the excess air and $\phi = (y - w)/4$ if $y > w$ and $\phi = 0$ if chlorine molar fraction is higher that hydrogen molar fraction in the fuel.

The pseudo Bond Graph models for the thermochemical processes are constructed starting from the reaction schemas and considering the mass and heat transfers within the reactor.

During the model construction phase, a difficult task was represented by the complex and non-linear reactions kinetics modelling with high influence on energetic stage of the process. This task was solved by introducing the multiport modulated element RS. The Bond Graph model from Fig. 1 is composed of one part that corresponds to chemical balances and one part corresponding to energy balance. The connection between theses two part, chemical and thermal, is accomplished by the bi-port resistive element $RS_{36,37}$. The first port corresponds to reaction kinetics based on reaction rate:

$$f_{36} = k_0 e^{-E/RT} C_{C_zH_yO_xCl_wS_vN_u} C_{O_2} C_{N_2} V$$

where k_0 is the pre-exponential factor, E is the activation energy, R - perfect gas universal constant, T - process temperature, V reactor volume and $C_{C_zH_yO_xCl_wS_vN_u}$, C_{O_2} and C_{N_2} are the concentration of $C_zH_yO_xCl_wS_vN_u$, O_2, N_2 elements. The reaction rate is:

$$r = k_0 e^{-E/RT} C_{C_zH_yO_xCl_wS_vN_u} C_{O_2} C_{N_2}$$

The non-linearity of f_{36} term is given both by the dependence on temperature T (e_{37}) according to Arrhenius low and by the reactants concentrations (e_2 fuel concentration, e_7 oxygen concentration and e_{12} nitrogen concentration).

The second port of RS element models the heat flow based on reaction heat and reaction kinetics:

$$f_{37} = (\Delta H) k_0 e^{-E/RT} C_{C_zH_yO_xCl_wS_vN_u} C_{O_2} C_{N_2} V$$

where ΔH is the heat of reaction.

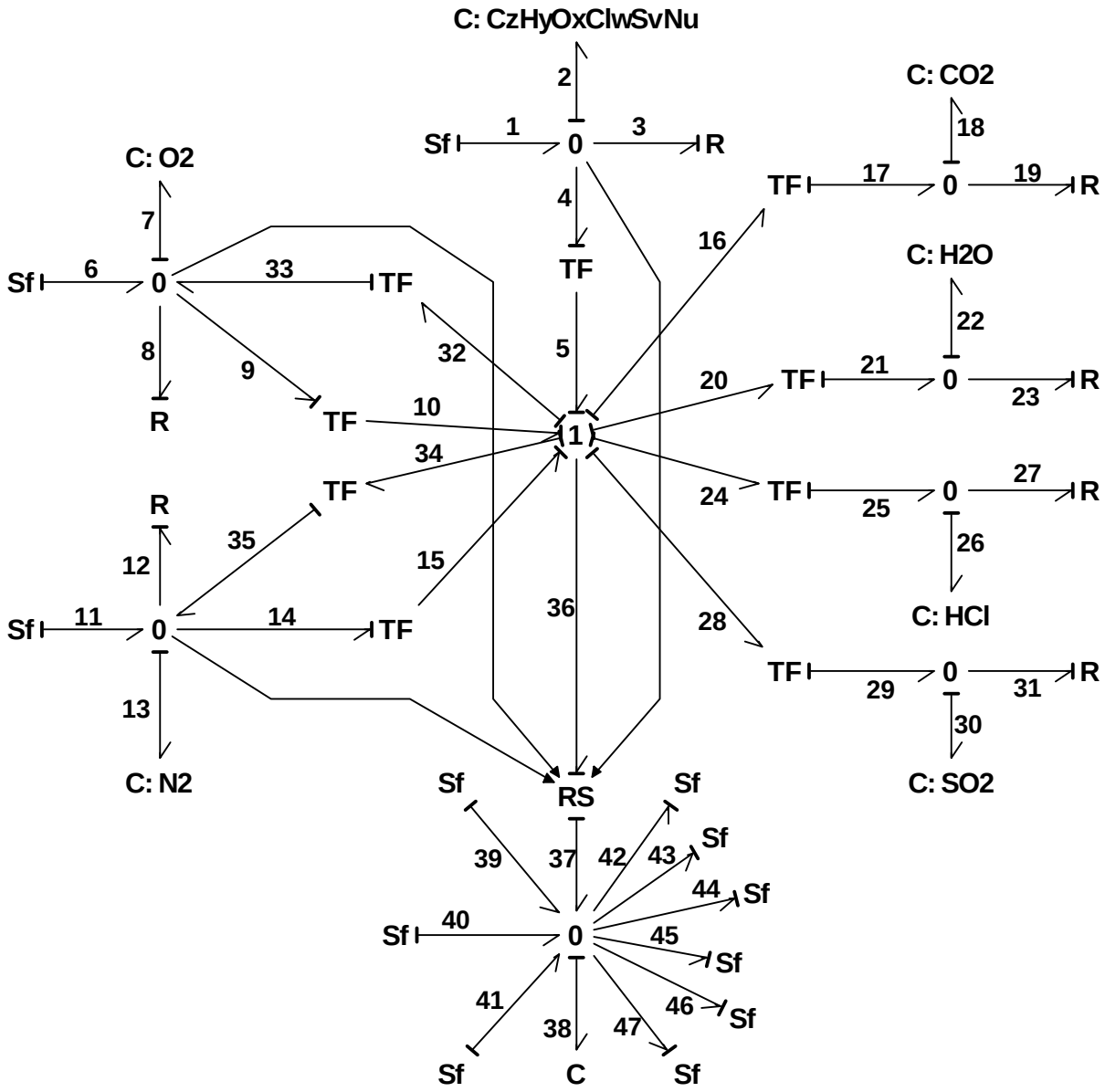

Fig. 1 Pseudo Bond Graph model of the process

At micro level the thermochemical processes using multi-component or mixed reactants are characterized by several chemical reactions that occur quasi-simultaneous with slightly different and inter-conditioned reaction rates. Thus, a product from a reaction becomes reactant for other, the reaction rate of the second reaction being conditioned both by previous reaction kinetic and the concentrations and partial pressures of all products in the process. Therefore, in the last section of the chapter a system composed of three inter-dependent reactions that corresponds to the combustion of a gas fuel mixture was modelled.

The results obtained through simulations proved a good correlation between the two parts of the process, chemical / energetic, respectively the evolutions of chemical species concentrations and process temperature.

The **last chapter** of the current work is dedicated to the study of Bond Graph methodology applicability in modelling the biotechnological processes in main bioreactors types ***representing an original and necessary contribution because the bioprocesses modelling through Bond Graph has not been studied till this moment***.

Due to chemical reactions in modelling process, it was used the same Bond Graph method as in previous chapter adapted to biochemical reactions particularities and keeping both the unitary characteristic and bases methodology advantages. In biotechnology the process main parameters are organic connected and modification of one of them induces others modification, characteristic that can be observed in the most of the biotechnological processes.

Bond Graph models were accomplished starting with processes reactions schemas – that do not represent stoichiometric relations as for the chemical reactions but qualitative relations – and using both base elements of Bond Graph methodology and pseudo bonds with effort and flow variables as concentrations and mass flows. Dynamic models corresponding to main biotechnological processes were obtained: microbial growth on limited substrate, aerobic microbial growth associated to enzymatic catalysis reaction and anaerobic fermentation for organic waste treatment.

To exemplify, the Bond Graph model (Fig. 2) associated to organic fraction from residual waste water treatment is presented with the complex reaction schema of 4 reactions and 10 components:

$$\begin{cases} S_1 \xrightarrow{\varphi_1} X_1 + S_2 + S_3 + S_4 + S_5 \\ S_2 \xrightarrow{\varphi_2} X_2 + S_5 + P_1 \\ S_3 \xrightarrow{\varphi_3} X_3 + S_2 + S_4 + S_5 \\ S_4 + S_5 \xrightarrow{\varphi_4} X_4 + P_1 \end{cases}$$

In this reaction schema S_i, i=1…4 represent the substrates: S_1 represents the glucose, S_2 the acetate, S_3 the propionic acid, S_4 the hydrogen, S_5 the inorganic carbon, X_1 represents acidogenic bacteria, X_2 acetoclastic methanogenic bacteria, X_3 represents the ionised hydrogen, X_4 the hydrogenophil methanogenic bacteria and P_1 represents the resulting product – methane CH_4.

Bond Graph model from Fig. 2 is made starting from the reaction schema together with phenomena occurring inside the bioreactor.

The half arrows direction in the Bond Graph model corresponds to reaction development, starting from component S_1 to components X_1, S_2, S_3, S_4 and S_5 for the first reaction, from component S_2 to components X_2, S_5 and P_1 for the second reaction, from S_3 to components X_3, S_2, S_4 and S_5 for the third reaction and respectively from S_4 and S_5 to X_4 and P_1 for the last reaction.

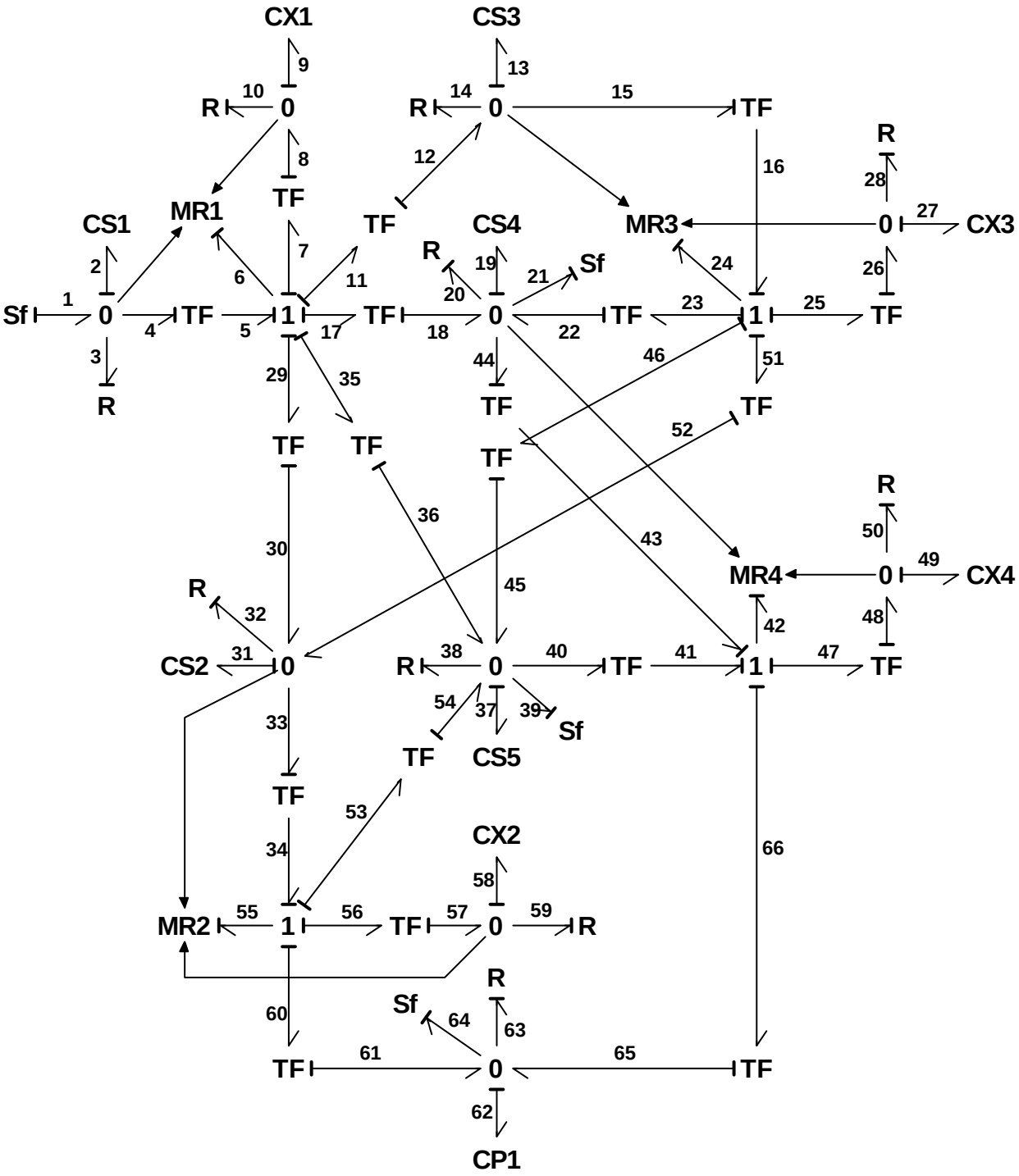

Fig. 2 Bond Graph model of the complete reaction schema
for biodegradation treatment process

During the dynamic model construction stage a difficult task was represented by the ***modelling of reactions kinetics, their complex and non-linear form being solved by introducing uniport or multiport resistive modulated elements MR***.

For each process type, the analytic and Bond Graph modelling was performed both for extended as for simplified process version. For the Bond Graph model the reaction schema and biochemical phenomena specific to each considered process was taken into account. Starting from this model, based on characteristic equations for both elements and junction structure was obtained the equation system representing the very mass balance equation system. Introducing the constructive and process characteristics of the system in mathematical terms the dynamic model was obtained, being validated by comparing to the model obtained using classic modelling methods. Again the models simulations results present evolutions of the process parameters identical to those obtained in the scientific main stream literature.

The biotechnological processes Bond Graph modelling is faster than classic one, allowing, by using 20sim modelling and simulation environment (product of Controllab Products B.V. Enschede, Netherlands), to obtain the time variation evolution for state variables. Moreover, starting from Bond Graph model the structural properties can be naturally established, which is a difficult task using classic modelling methods.

The current work answers the present issues in the field of Bond Graph modelling adding a necessary contribution in thermochemical and biotechnological processes modelling through the development of base methodology.

The study undertaken within this work highlighted the importance of modelling using Bond Graph methodology for technological processes mainly due to mechanical, electrical, thermal and chemical phenomena coexistence. Compared to classic modelling, depending on modelled system complexity and performed modifications, through this study was demonstrated the possibility to add or eliminate elements in Bond Graph structure according to physical systems modifications without being necessary to start over on whole modelling algorithm. This characteristic has an important applicability in modelling the thermo chemical and biotechnological processes due to their non steady state evolution imposed by time variation of some process parameters. The elements, concepts and structures developed and validated in this work are the base for Bond Graph versatility and application extension in technological systems modelling, providing a tool for academic, research and industrial level.