

2. Basic Element of Coupled Bond Graph

Bond graph models are network type models which are composed of multiports related by power bonds representing the (acausal) identity between pair of conjugated variables (named effort and flow) whose product is the instantaneous energy flow between the multiport elements. The multiport elements represent storage (**C-element**) (as compliance for instance or volume), inertia (**I-element**) (electrical inductance and mechanical inertia), energy dissipation (**R-element**) (electrical, mechanical or thermal friction), balance and continuity equations (the **0- and 1-junctions**) or inter-domain coupling (the **TF transformer** and **GY gyrator** elements). Finally to reproduce the architecture of the global system to be modelled, bond graph elements (R, C, I,..) are interconnected by a "0" junctions when they have a common effort and by "1" junction if their flow is the same.

In process engineering processes, several phenomena (chemical, thermal and fluidic) are coupled. In addition to matter transformation phenomena, chemical and electrochemical processes involve additional complexity in the modelling task, since the mass that flows through the process carries the internal energy which is stored in it, and which is thus transported from one location to another in a non-dissipative fashion. Power variables are thus in vectorial form:

$$E = [e_h \ e_t \ e_c]^T, F = [f_h \ f_t \ f_c]^T \quad (1)$$

where e_h , e_t and e_c represent respectively the thermal effort (specific enthalpy h or the temperature T), the hydraulic effort (the pressure P), and the chemical effort (the chemical potential μ , chemical affinity A or the concentration c). f_h , f_t and f_c represent respectively the thermal (or entropy) flow (by conduction \dot{Q} or by convection \dot{H} i.e. enthalpy flow), hydraulic flow (mass flow \dot{m} or volume flow \dot{V}) and chemical flow (molar flow \dot{n}).

Consider a thermofluid process (Figure 2 (a)) which consists of a pump (considered as a flow source) fulfilling a heated tank where a bottom pressure is measured by the sensor P_m , and the average temperature of the fluid is indicated by T_m . The coupled bond graph model in integral causality is given by Figure 2 (b). The two ports C_{ht} represents the coupled thermal and hydraulic energy of the stored fluid (considered here in under saturated state) is decoupled into thermal and hydraulic capacity C_t , and C_h . $Sf : \dot{Q}_m$, $Sf : \dot{m}_m$, and $Se : T_m$ represent,

respectively, thermal flow source, inlet mass flow, and the temperature of the incoming fluid (considered constant). The coupling is modelled by the fictive R_c element in the thermal bond.

Another complexity can be added taking into account transformation of matter in chemical phenomena. The corresponding bond graph model is given by Figure 3. The mixture of mass flow \dot{m}_m is considered multicomponent with n species. The n transformers with $1 / M_i [Kg.mole^{-1}]$ as modulus used to transform massic flow \dot{m}_m to molar flow $\dot{n}_{i,m}$ of i^{th} specie:

$$\dot{n}_{i,m} = \frac{\dot{m}_m}{M_i} \quad (2)$$

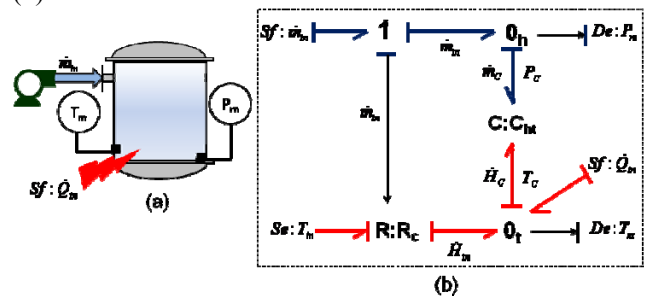


Fig. 2. Heated tank (a) and its BG model in integral causality (b)

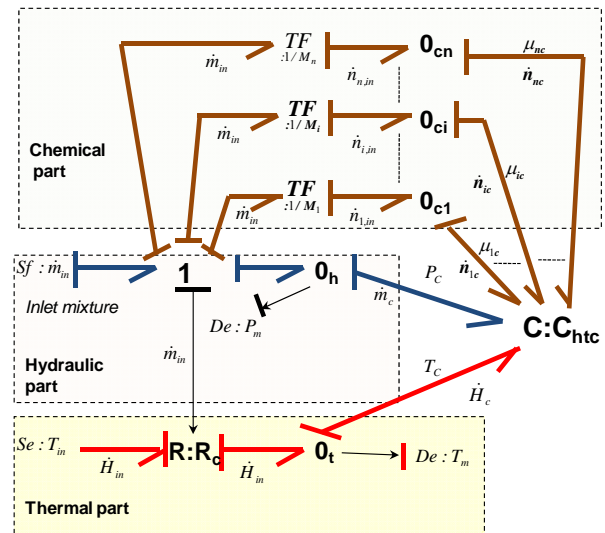


Fig. 3. Bond graph model with three coupled energies

The state equation form $x = f(x, u)$ well suited for control analysis, can be systematically deduced from a bond graph in a linear or non linear form. The input vector u is represented in a bond graph by the sources (Se and Sf), the measured variables are effort and flow detectors. The state vector is composed by the energy variables

stored by C (general displacement) and I elements (impulse). The state vector does not appear on the Bond Graph, but only its derivative: The dimension of the state vector is equal to the number of C and I elements in integral causality. In the given dynamic model, there are $n+2$ state variables: $x = [m_c H_c n_{cn} \dots n_{cn}]$. They represent storage of number of mole for $n+2$ species, total mass m_c and internal energy of the mixture H_c .

3. Uncertain Coupled Bond Graph

3.1 Uncertain Bond Graph Interest

Various bond graph based qualitative and quantitative [5], FDI approaches have been developed to detect and isolate faults in single or piece-wise single energy domains, but none deal with FDI of coupled (energetic and transformation phenomena) nonlinear systems.

Among recent works that deal with parameter uncertainties modeling using bond graph approach, in [6], the authors proposed to construct in a systematic manner a bond graph from another bond graph using standard interconnection form, which is called the associated incremental bond graph (IBG).

In [7]-[8], authors proposed two methods for modelling uncertainties by using bond graph approach, applied on Electromechanical and thermodynamic systems (vehicle, test bench and steam generator). The first method is based on describing parameter uncertainties as bond graph elements, and the second method introduces the LFT form for uncertainties modelling. Here, this problem is addressed using the linear fractional transformation (LFT) paradigm.

After the pioneering work of Oster and Perelson, it has been mainly used for membrane processes some reaction processes and some electrochemical processes [9]-[10]. Bond graph modeling has been used for hydraulic and thermal domain in chemical reactor but not for monitoring and observing kinetic and thermodynamic evolution of chemical mixture. Thus, uncertain bond graph modeling of chemical reaction are not treated until now in literature and diagnosis of chemical reaction is an open research work.

3.2 BG-LFT Form

The principle of the uncertainties representation using LFT consists in building the uncertain system in the form of a looping between the increased invariant system M , whose parameters are defined perfectly, and a block of uncertainty, noted Δ , gathering various uncertainties, Figure 4. Setting of LFT form requires that the system must be reachable and observable. These properties are necessary conditions for the monitoring ability of the system.

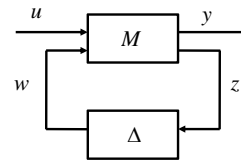


Fig. 4. LFT representation

The interconnection structure induces the following state equations:

$$\begin{cases} w = -\Delta z \\ \dot{x} = Ax + B_1 w + B_2 u \\ z = C_1 x + D_{11} w + D_{12} u \\ y = C_2 x + D_{21} w + D_{22} u \end{cases} \quad (3)$$

where $x \in \mathfrak{R}^n$ the state vector, $u \in \mathfrak{R}^m$ the inputs vector, $y \in \mathfrak{R}^p$ the outputs vector. $w \in \mathfrak{R}^l$ and $z \in \mathfrak{R}^l$ are, respectively, the auxiliary input and output vectors. n, m, l et p are positive entières. $A, B_1, B_2, C_1, C_2, D_{11}, D_{12}, D_{21}, D_{22}$ are appropriate ranks matrices.

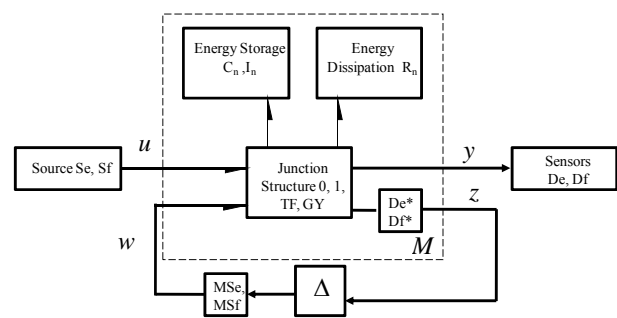


Fig. 5. BG-LFT representation

In LFT bond graph representation, parameters uncertainties are represented under multiplicative form at the level of bond graph component. The method consists in replacing each uncertain element by its BG-LFT. BG-LFT representation is shown in Figure 5.

The advantage of approach BG-LFT compared to an approach of LFT state is summarized in two points:

complexity in the model construction and the uncertainties structure on the model [4].

Modeling of bond graph elements $i \in \{R, I, C, TF, GY\}$ in the LFT form consists in decoupling the nominal element $i_n \in \{R_n, I_n, C_n, TF_n, GY_n\}$ part from its uncertain part $\delta_i i_n \in \{\delta_R R_n, \delta_I I_n, \delta_C C_n, \delta_{TF} TF_n, \delta_{GY} GY_n\}$, with δ_i is a multiplicative uncertainty on the parameter i . In the combined BG-LFT representation, the parameter uncertainties are explicitly represented under multiplicative form for each bond graph element. The additive uncertainties of the parameters are related to their multiplicative values by the following relations: $\delta_i = \frac{\Delta i}{i_n}$,

where Δi is the additive uncertainty values on the bond graph element i .

The principle of this modeling consists in representing the influence of the parameter uncertainty, by a fictive effort or flow input ($MS_e : w_i$ or $MS_f : w_i$), modulated by $\delta_i(i_n e_i)$ or $\delta_i(i_n f_i)$. Details on this modelling procedure are given in [8].

In chemical processes, to explain the modelling in LFT form using the bond graph, let us consider the Multiport \square , we know that the R-elements dissipate power and that this power comes out as heat. So including thermal effects, an R-element becomes an irreversible and power conserving structure. It is denoted as multiport \square (see Figure 6 (a)). So power can flow only as indicated by the half arrows, and not backwards. In other words it cannot become negative. So, when we are not interested in thermal effects, we speak of R-elements and multiport-R, otherwise of multiport- \square . Regarding the multiport \square , it can have bonds with several strands as shown on Figure 6 (b). With multiport \square , irreversibility and energy conservation of multiport R are as follows: with several strands, only the sum of the non thermal bonds must be positive, but in single strands power can become negative as long as it is more positive in others. One can also say that power in the thermal bond must be always positive.



Fig. 6. Element (a) and Multiport \square

In a chemical reaction, the product of chemical affinity A by the global reaction rate J is a power. The thermal loss (transformation of chemical to thermal energy) is modeled

by an active resistance Multiport \square (a resistance which generates entropy) [11]. The multiport absorbs chemical power $A \times J$ and produces an equivalent quantity in thermal power $T \times S$. Thus, a RS-field is used as a link between the mass and energy parts of the reactor vessel subsystem. It is a two-port element connecting the molar and energy balances.

The characteristic law of Multiport \square in resistance causality with uncertainty can be written as follows:

$$\begin{aligned} \dot{S} &= \Phi(\square_n, A)(1 + \delta_{1/\square}) \\ &= \Phi(\square_n, A) + \delta_{1/\square} \Phi(\square_n, A) \\ &= \dot{S}_n + \dot{S}_{inc} \end{aligned} \quad (4)$$

The effort A is known at the entry of the multiport \square . $\dot{S}_n, \dot{S}_{inc}, \delta_{1/\square}$ represent, respectively, the nominal value, the multiplicative uncertainty. $\Phi(\square_n, A)$ is the global reaction rate and is written as

$$\Phi(\square_n, A) = r_f \left(1 - \exp\left(-\frac{A}{RT_r}\right) \right) V \quad (5)$$

where the reaction $r_f = k_0 \exp\left(\frac{-E_a}{RT_r}\right) \prod C_i^{v_i}$ represents non linear term which depends on reactional temperature T_r , according to Arrhenius equation, and concentrations ($C_i = \frac{n_i}{V}$). R is a universal gas constant, E_a is the activation energy of the reaction and k_0 is the pre-exponential factor.

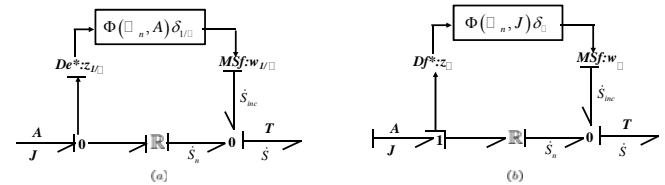


Fig. 7. Multiport \square in resistance causality using the LFT form (a)
 Multiport \square in conductance causality using the LFT form (b)

The characteristic law of R \square element in conductance causality is given as follows:

$$\begin{aligned} \dot{S} &= \Phi(\square_n, J)(1 + \delta_{\square}) \\ &= \Phi(\square_n, J) + \delta_{1/\square} \Phi(\square_n, J) \\ &= \dot{S}_n + \dot{S}_{inc} \end{aligned} \quad (6)$$

The flow J is known at the entry of the multiport \square . In the next section will be considered the use of coupled bond graph for FDI design.

4. Fault Indicators Generation from Bond Graph

In this paper, a bond graph methodology is used to synthesis a robust FDI method for nonlinear system in presence of parameter uncertainties, Figure 8.

Parametric uncertainties are explicitly appears on the BG, one can automatically generate the robust ARR for the uncertain system by decoupling the nominal and the uncertain parts; residuals correspond to the ARR nominal part, while the residual thresholds represents the ARR uncertain parts.

The main advantages of the bond graph model in LFT form for robust diagnosis are given as follows:

- Introduction of the uncertainties on the nominal model, does not affect the causality and the structural properties of the BG elements;
- Representation of all uncertainties (i.e. structured and unstructured);
- Uncertain part is perfectly separated from the nominal part;
- Parameter uncertainties are easily evaluated.

This FDI method is summarized by the following steps:

- i) Modeling of studied system using bond graph tool with standard LFT form;
- ii) Generation of Analytical Redundancy Relations (ARRs) from the uncertain model by decoupling the nominal and the uncertain parts. Residuals correspond to the ARR nominal part, while their adaptive thresholds represent the ARR uncertain parts;
- ii) Residual' sensitivity analysis is done by using the ARR uncertain part.

5. Fault Indicators Generation from Bond Graph

5.1 Case Study: A Chemical Reactor

5.1.1 Process Description

Let us consider an adiabatic Continuous Stirred Tank Reactor, where the exothermic reversible reaction is occurred. This reaction is defined as follows:

$$n_A A \xrightleftharpoons[k_A]{k_A} n_C C \quad (7)$$

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$$n_A A \xrightleftharpoons[k_A]{k_A} n_C C \quad (7)$$

where ν_i (for $i=A, C$) are the stoichiometric coefficients.

In our case these coefficients are equal to one.

The technological diagram of reactor system is depicted in Figure 9. The supply system (component A) consists of a storage tank and a pump. The level regulation is guaranteed by the means of a PI regulator acting on a centrifugal pump which supplies continuously the tank.

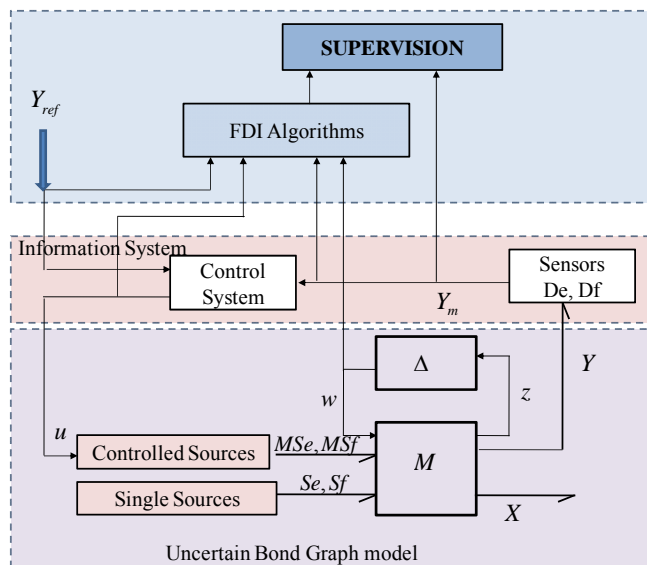


Fig. 8. Representation of the robust FDI scheme using bond graph tool

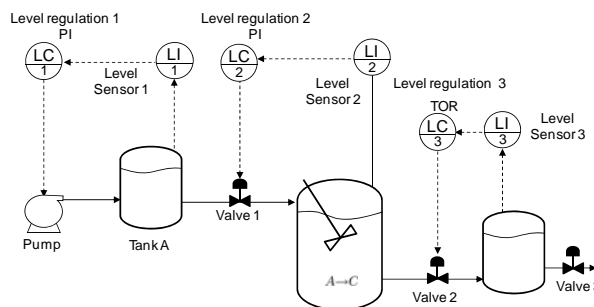


Fig. 9. Technological diagram of the process

The level controller in the reactor is ensured by a regulator which acts on a valve at the reactor input. The tank containing the components (C, A) is controlled in level by a regulator which acts a self-closing valve on the outlet side of the reactor.

5.1.2 Word Bond Graph

The modelling hypotheses are, the reactor is perfectly stirred so that temperature and concentrations of different chemical species are homogeneous in all the reaction mixture, the reaction mixture is composed of one

homogeneous liquid phase, and no phase change is considered, the volume of the liquid in the tank is constant. For illustration of developed method and because of limited space, we consider only the main component of the system: reactor vessel especially chemical domain.

The word bond graph model is presented in Figure 10. This model is decomposed into several modules, linked by a pair of pseudo power variables (effort-flow). To simplify the process modelling, we introduced bond graph model of reactor vessel which is composed of several parts corresponding to multi-energy domains.

The used pseudo power variables (effort-flow) are: pressure-mass flow (P, \dot{m}) , temperature-enthalpy flow (T, \dot{H}) in the case of convection, and temperature-thermal flow (T, \dot{Q}) in the case of conduction, chemical potential-molar flow (μ, \dot{n}) , chemical affinity-reaction velocity (A, J) .

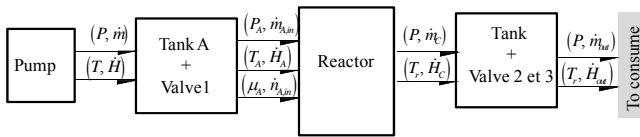


Fig. 10. Word pseudo-bond graph of the chemical reactor

5.1.3 Pseudo Bond Graph Model

The bond graph model is given (Figure 11). This part includes chemical subsystem in reactor vessel. The bond graph transformers $TF:1/\nu_A$ and $TF:1/\nu_C$ represent a chemical transformation. Their modulus is the stoichiometric coefficients (the chemical affinity A represent the driving force in reactor vessel).

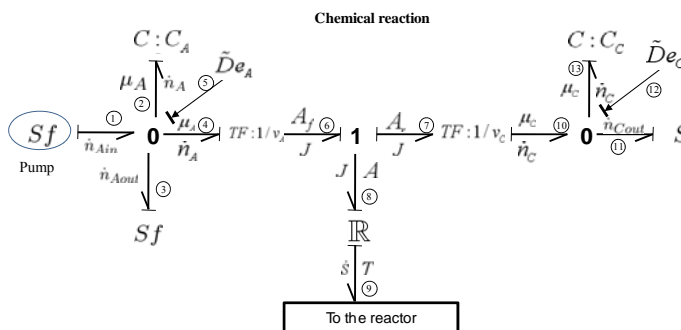


Fig. 11. BG determinist model in preferred derivative causality of chemical domain

In the chemical domain the 0-junctions represent the molar balance of each component (A, C). 1-junction is used to

represent the equality of the molar reaction flows of the different substances involved.

Thus, a \square -field is used as a link between the mass and energy parts of the reactor vessel subsystem. It is a two-port element connecting the molar and energy balances.

Modelling of bond graph elements $i \in \{C_A, C_C\}$ and multiport $\{\square\}$ in the LFT form consists in decoupling the nominal element $i_n \in \{C_{A,n}, C_{C,n}, \square_n\}$ part from its uncertain part $\delta_{i_n} \in \{\delta_1 C_{A,n}, \delta_2 C_{C,n}, \delta_3 \Phi(\square_n, A)\}$, with δ_i is a multiplicative uncertainty on the parameter i .

The determinist and uncertain bond graph model of the chemical domain are respectively given in Figures 11 and 12. The symbols $\tilde{D}e$ and $\tilde{D}f$ correspond to virtual sensors. They are used to distinguish the real measurements from the fictive ones.

The storage of chemical energies is modelled by the bond graph elements $C:C_A$ and $C:C_B$. Then the following equation is deduced from the junction 0 of the bond graph determinist model in derivative causality:

$$\begin{cases} \dot{n}_A = \frac{V}{RT} \exp\left(\frac{\mu_A - \mu_A^0}{RT}\right) \dot{\mu}_A \\ \dot{n}_C = \frac{V}{RT} \exp\left(\frac{\mu_C - \mu_C^0}{RT}\right) \dot{\mu}_C \end{cases} \quad (7)$$

where μ_A^0 is standard chemical potential.

In general case, the previous equations becomes

$$\dot{n}_i = C_i \frac{d\mu_i}{dt} \quad (8)$$

where \dot{n}_i is the reaction output' molar flow. μ_i is chemical potential inside the reaction. C_i represents the chemical capacity of the reaction and can be expressed as follows:

$$C_i = \frac{V}{RT} \exp\left(\frac{\mu_i - \mu_i^0}{RT}\right) \quad (9)$$

The relation between $C_{i,n}$ and δ_{C_i} is given by the following expression:

$$C_i = C_{i,n} + \delta_{C_i} C_{i,n} \quad (10)$$

where $C_{i,n}$ is the nominal value of C_i .

The modulated input w_i ($i=2,3$) in Figure 12 corresponds to an effort variable deduced from δ_{C_i} and expressed by the following equation:

$$w_i = -\delta_{C_i} C_{i,n} \frac{d\mu_i}{dt} \quad (11)$$

w_i is taken with a negative sign, because it is considered as a fictive flow input' source.

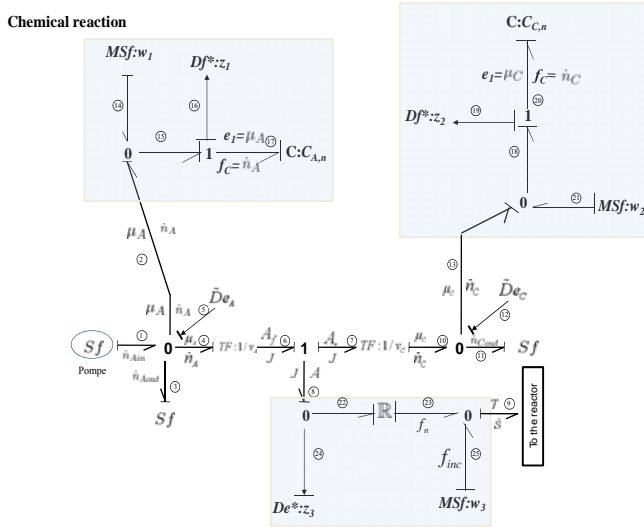


Fig. 12. BG-LFT uncertain model in preferred derivative causality

5.1.3 Design of Supervision System

A method to derive ARR from bond graph models by applying the causality inversion algorithm, have been presented in [4], which use structural and causal properties.

Determinist ARR's Generation: The ARR's are deduced from junctions 0 that contain detectors on the nominal bond graph model of Figure 12. The unknown variables f_2 and f_4 are eliminated using covering causal paths from detectors to unknown variables.

From first junction 0

$$r_1 = f_1 + f_4 - f_3 - f_2 = 0 \quad (12)$$

with $f_1 = Sf = \dot{n}_{Ain}$, $f_3 = Sf_{out}$, $f_2 = C_A \frac{de_2}{dt}$

$$f_4 = v_A f_6 = v_A J = v_A \Phi(\square, A) = v_A r_f \left(1 - \exp\left(\frac{A}{RT_r}\right) \right) V$$

where $\Phi(\square, A)$ is given by the equation (5).

f_2 is calculated (eliminated) from the following causal paths $f_2 \rightarrow \Phi_{C_A} \rightarrow e_2 \rightarrow \tilde{D}e_A : \mu_{A,m}$

The first ARR, r_1 , is deduced from equation (12) and is given as

$$\begin{aligned} r_1 &= \dot{n}_{Ain} + v_A \Phi(\square, A) - Sf_{out} - C_A \frac{d\tilde{D}e_A}{dt} \\ &= \dot{n}_{in} \frac{C_{Ain}}{\rho_A} + v_A \Phi_R(n_A, m, H) - \dot{m}_{out} \frac{n_A}{m_{me}} - \dot{n}_{A,m} = 0 \end{aligned} \quad (13)$$

with $m_m = \rho V = \rho SL_m$ (S sectional surface of the reactor)

$$\text{and } \dot{n}_{A,m} = \frac{V}{RT_r} \exp\left(\frac{\mu_{A,m} - \mu_A^0}{RT_r}\right) \dot{\mu}_{A,m}.$$

From second junction 0

$$r_2 = f_{10} - f_{11} - f_{13} = 0 \quad (14)$$

and from the constraint in equation (14), the second ARR, r_2 , is given by

$$\begin{aligned} r_2 &= f_{10} - f_{11} - f_{13} = v_C \Phi(\square, A) - Sf_{out} - C_C \frac{d\tilde{D}e_C}{dt} \\ &= \dot{m}_{out} \frac{n_C}{m_{me}} - v_C r_f \left(1 - \exp\left(\frac{A}{RT_r}\right) \right) V - \dot{n}_{C,m} = 0 \end{aligned} \quad (15)$$

The fault in chemical domain (appearance of secondary event: release of toxic or explosive material, etc.) related to transformer phenomenon can be detected by using the first and the second ARR.

Robust ARR's Generation:

In this section, the ARR's are generated for nonlinear systems, using bond graph approach in the LFT form. The aim of the robust diagnosis for the presented chemical reaction is to detect and isolate a chemical fault situation (appearance of secondary reaction when the reaction takes place; undesirable product and runaway of the reaction) in presence of parameter uncertainties. This fault corresponds to the increase of the reaction velocity and chemical affinity, which is distinguished from the parameter uncertainties.

The chemical reaction model in the LFT form with derivative causality, after sensors dualization is given in Figure 12. The fictive inputs w_i ($i=1, \dots, 3$) are related with the fictive outputs z_i ($i=1, \dots, 3$) and expressed in the system of (16)

$$\begin{cases} w_1 = -\delta_1 z_1; z_1 = \dot{n}_A = C_A \frac{d\tilde{D}e_A}{dt} = C_A \frac{d\mu_A}{dt} = \frac{V}{RT} e^{\left(\frac{\mu_A - \mu_A^0}{RT}\right)} \frac{d\mu_A}{dt} \\ w_2 = -\delta_2 z_2; z_2 = \dot{n}_C = C_C \frac{d\tilde{D}e_C}{dt} = C_C \frac{d\mu_C}{dt} = \frac{V}{RT} e^{\left(\frac{\mu_C - \mu_C^0}{RT}\right)} \frac{d\mu_C}{dt} \\ w_3 = \delta_3 \Phi(\square, A) z_3; z_3 = e_6 = A_f = v_A \mu_A \\ \quad \quad \quad = v_A \left(\mu_A^0 + RT \text{Log} \left(\frac{\int \dot{n}_A dt}{V} \right) \right) \end{cases}$$

where δ_1 and δ_2 represent, respectively, multiplicative uncertainties on the energy accumulation of reactant A and product C (leads to uncertainties in heat-storage capacity). δ_3 is the multiplicative uncertainty on the reaction velocity (leads to uncertainties in activation energy, pre-exponential factor, enthalpy...).

The two parts of the ARR generated from chemical reaction model with parameter uncertainties of Figure 12 are given by equations (12) and (15) where r_1 and r_2 represent the ARRs nominal parts that describe the system operating. a_1 and a_2 (the ARRs uncertain part) represent the intake reduced by the parameter uncertainties such as flow or effort which affect the residuals. It is described by the sum of fictive input values and is used to calculate the normal operating thresholds.

$$\begin{cases} a_1 = |w_1| + |v_A w_3| \\ a_2 = |w_2| + |v_C w_3| \end{cases} \quad (17)$$

Uncertain ARR part cannot be quantified perfectly, it is evaluated to generate a normal operation' threshold which satisfies the following inequality:

$$-a \leq ARR \leq a \quad (18)$$

5.1.4 Simulation Results

The chemical system is instrumented with the following sensors. The mixture temperature inside the tank De : Tm1, the level inside the tank De : Lm1, the flow sensor (Df : Fm1) is used to measure the amount of mixture leaving the tank. The water flow in the cooling circuit can be measured using the flow sensor (Df : Fm2). The output control signal of each controller is considered as a known value.

Figure 13 show respectively the residuals r_1 and r_2 without faults.

Fault scenario: Appearance of the secondary reaction: It is supposed now for example that the cooling system is never failing and that the exits of the regulators and the sensors are always correctly measured. A sudden appearance of secondary product occurs between 30 and 60 min. Indeed, to stop the evolution of the secondary reaction and to eliminate these effects in real-time, it is necessary to add a reagent able to eliminate the undesirable products. As can be seen in Figure 14, the appearance of undesirable product is detected perfectly by the residual evolution. The fault is detected perfectly, as it is alarmed by two residuals r_1 and r_2 , and not by the other residuals. The thresholds of normal operation are given with dot lines.

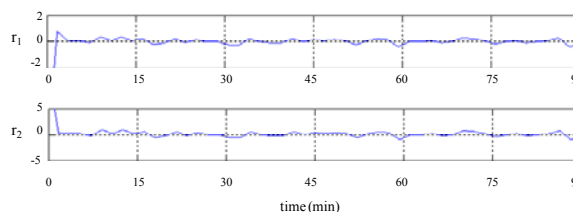


Fig. 13. Residual evolutions of normal system

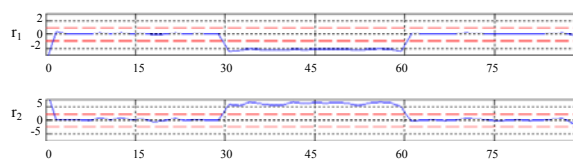


Fig. 14. Residual evolutions of faulty system

In order to explain the appearance of secondary reaction; for example, appearance of undesirable product E which modify reaction dynamics. Namely an unmodeled side reaction, is added to the simulation model; in detail the reaction scheme becomes:



and consequently the mass balance and the fault indicator will be modified. The RRAs (r_1 and r_2) should add the term $v_E \mu_{E,m}$ and can not be equal to zero.

6. Conclusions

In this paper, a robust FDI with respect to parameter uncertainties is given using bond graph modelling approach in the LFT configuration. The robust ARR are generated directly from a bond graph model. This approach is study for complex systems where numerical values of parameters are not available. The obtained results are validated using real process (continuous reactor). The proposed FDI method witch can detect kinetic and thermodynamic drift of chemical reactors due to appearance of secondary reaction. The performances obtained are acceptable.

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