On bond graph modelling of thermo-chemical processes

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Abstract: *The paper presents an approach of the Bond Graph modelling applied to thermo-chemical processes. The proposed work focused on combustion process kinetics with respect to reactant and reactor input data. The model provides information on the time variation of the heat of reaction, reaction products concentration, and reactants concentration / accumulation, based on global mass and energy balance of the process. The basic reaction between solid carbon and oxygen was considered to model the combustion solid fuel. The model can be used as base for the development of multi-component combustion reactions with enhanced thermal transfer.*

Key words: *thermo-chemical processes, Bond Graphs, modelling.*

Introduction

Both in chemical industry and energy sector, the thermo-chemical processes are widely used for derived substances synthesis and power generation from various fuels. The main processes are oxidative and reductive type. This study focused on oxidation processed with heat generation using both solid and gaseous fuels.

The thermo-chemical processes use highly exothermic or endothermic chemical reaction with the generation of heat or new products that can be used in industrial applications. One of the most used thermo-chemical process is the combustion that consists in a sequence of oxy-reductive chain reactions with highly exothermic overall energy balance. The useful effect is represented by the heat generated by the process as function of physical-chemical properties of the feed product and reactions stoichiometry (Tilmann, 1991).

Modelling of thermo-chemical processes is a difficult task. An alternative simplified modelling to the dedicated analytical approach is the Bond Graph modelling method.

Bond Graph method was first introduced by Paynter and further developed by Rosenberg and Karnopp in (Karnopp et al., 1990), and Thoma in (Thoma, 1990).

Over the last four decades there have been a lot of publications regarding the theory and application of Bond Graphs in different engineering domains. The Bond Graph approach is a powerful tool for modelling, analysis and design of different kind of systems, such as electrical, mechanical, hydraulic, thermal, chemical (Thoma et al., 2000) etc. This method provides a uniform manner to describe the dynamical behaviour for all types of physical systems and illustrates the exchange power in a system, which is normally the product between the effort and flow variables in the true Bond Graph. Besides this representation there is another one, in which the product effort-flow does not have the physical dimension of power, called pseudo Bond Graph (Thoma et al., 2000). Pseudo Bond Graphs are more suitable for chemical systems due to the physical meaning of the effort and flow variables. The advantages of Bond Graph modelling are the following: offers a unified approach for all types of systems; allows to display the exchange of power in a system by its graphical representation; due to causality assignment it gives the possibility of localization the state variables and achieving the mathematical model in terms of state space equations in an easier way than using classical methods; provides information regarding the structural properties of the system, in terms of controllability and observability.

Bond Graph methodology

Bond Graph method uses the effort-flow analogy to describe physical processes. A Bond Graph consists of subsystems linked together by lines representing power bonds. Each process is described by a pair of variables, effort e and flow f, and their product is the power. The direction of power is depicted by a half arrow. In a dynamic system the effort and the flow variables, and hence the power fluctuate in time.

One of the advantages of Bond Graph method is that models of various systems belonging to different engineering domains can be expressed using a set of only nine elements. A classification of Bond Graph

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elements can be made up by the number of ports; ports are places where interactions with other processes take place. There are one port elements represented by inertial elements (I), capacitive elements (C), resistive elements (R), effort sources (Se) and flow sources (Sf), two ports elements represented by transformer elements (TF) and gyrator elements (GY), and multi ports elements - effort junctions (J0) and flow junctions (J1). I, C, and R elements are passive elements because they convert the supplied energy into stored or dissipated energy. Se and Sf elements are active elements because they supply power to the system, and TF, GY, 0 and 1-junctions are junction elements that serve to connect I, C, R, and source elements and constitute the junction structure of Bond Graph model. The concept of causality is an important concept embedded in Bond Graph theory. This refers to cause and effect relationship. Thus, as part of the Bond Graph modelling process, a causality assignment is implicitly introduced (Karnopp et al., 1990; Thoma, 1990).

Causality assignment is independent of the power flow direction. This leads to the description of Bond Graphs in the form of state – space equation. The sources (Se and Sf) have fixed causality, the dissipative element (R) has free causality depending on the causality of the other elements of Bond Graph, and the storage elements (I, C) have preferential causality, that is integral causality or derivative causality, but it is always desirable that C and I elements to be in integral causality. Transformers, gyrators and junction elements have constrainedly causality.

Besides the power variables, two other types of variables are very important in describing dynamic systems and these variables, sometimes called energy variables, are the generalized momentum p as time integral of effort and the generalized displacement q as time integral of flow (Karnopp et al., 1990).

Bond Graph modelling of the combustion process

Combustion represents the complete conversion into CO_2, H_2O, HCl, SO_x, NO_x of organic mater at temperatures between 750 °C – 1200 °C and pressures 0.7 – 1.3 bar. There are also combustion processes conducted at high temperatures and under different pressure conditions that can reach 2200 °C for specific applications only. The main reactants of the combustion reactions are carbon, hydrogen, sulphur, nitrogen, chlor and oxygen. The combustion processes optimization to increase the thermal-chemical conversion efficiency and to reduce the pollutant emissions requires kinetic models of the chemical reactions. The fuel/ oxidizer ratio, reaction products and reaction heat represent essential data for the control and operation of combustion processes (Tilmann, 1991).

Using the Bond Graph method, we will derive a model of the combustion process (1).

$$C + O_2 \xrightarrow{r} CO_2 \tag{1}$$

In order to model this kind of process, pseudo Bond Graph method is more appropriate because of the meaning of variables involved – effort (concentration) and flow (molar flow). This offers a flexible way to manage the material balances is terms of differential equations without losing the advantages of true Bond Graphs.

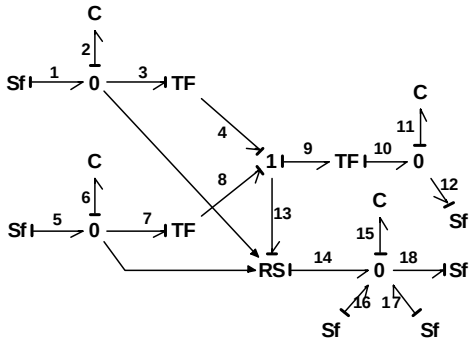

Fig. 1. Pseudo Bond Graph model of the process.

In the reaction scheme (1) we will denote the carbon element with *A*, the oxygen element with *B* and the carbon dioxide with *D*.

From the reaction scheme (1), and considering the mass transfer through the reactor the pseudo Bond Graph model of the thermo-chemical process of combustion is achieved. This model is presented in fig. 1. The directions of the half arrows in the Bond Graph correspond to the progress of the reaction, going out from the components *A* and *B* towards *D*.

In Bond Graph terms, the chemical part is represented by three 0-junctions that are in fact the mass balances of the elements involved in the reactor: $0_{1,2,3}$ (mass balance for carbon), $0_{5,6,7}$ (mass balance for

oxygen), and $0_{10,11,12}$ (mass balance for carbon dioxide). The second part of the Bond Graph model corresponds to the energy balance of the reaction and it is represented by a 0-junction, $0_{14,15,16,17,18}$, connected to the chemical part of the model through an RS element. This element is in fact a two port R element that includes thermal effects. One port is used to model the reaction kinetics through the rate of reaction that is a nonlinear term depending on the process temperature, activation energy related by a first order kinetics law of Arrhenius. This term can be represented by the relationship between effort and flow:

$$f_{13} = k_o e^{-E/RT} ABV \tag{2}$$

where k_0 is the pre-exponential factor, E is the activation energy [kJ·mol^{-1}], R is the perfect gas constant [kJ/kmolK], T is the process temperature [K], V is the reactor volume [m^3] and A, B are the concentrations of the similar elements [mol/m^3]. The process temperature T used in this equation is computed in the energetic part of the model.

The same element models at the second port the heat flow based on the heat of reaction and reaction kinetics.

$$f_{14} = (\Delta H) k_o e^{-E/RT} ABV \tag{3}$$

where ΔH is the heat of reaction [kJ/mol].

The constitutive relations of these junctions are characterized by the equality to zero of the sum of flow variables; therefore, the next relations are obtained: $f_{15} = f_{14} + f_{16} + f_{17} - f_{18}$, $f_2 = f_1 - f_3$, $f_6 = f_5 - f_7$, and $f_{11} = f_{10} - f_{12}$.

Thus, the accumulations of carbon, oxygen and carbon dioxide in the reactor are represented by bonds 2, 6 and 11, and they are modelled using capacitive elements C. The constitutive equations of C-elements are:

$$e_2 = \frac{1}{C_2} q_2 = \frac{1}{C_2} \int_t (f_1 - f_3) dt \tag{4}$$

$$e_6 = \frac{1}{C_6} q_6 = \frac{1}{C_6} \int_t (f_5 - f_7) dt \tag{5}$$

$$e_{11} = \frac{1}{C_{11}} q_{11} = \frac{1}{C_{11}} \int_t (f_{10} - f_{12}) dt \tag{6}$$

where C_2, C_6 and C_{11} are the parameters of C-elements: $C_2 = C_6 = C_{11} = V$.

The reactants input flows were modelled by two flow sources Sf_1 and Sf_5 and the stoichiometric coefficients were modelled using the transformer elements $TF_{3,4}$, $TF_{7,8}$, and $TF_{9,10}$. It was also used a source flow element Sf_{12} to in order to model the carbon dioxide outflow rate. From the constitutive relations of TF elements:

$$f_3 = k_{3,4} f_4, \quad f_7 = k_{7,8} f_8, \quad f_{10} = f_9 / k_{9,10}$$

with $k_{3,4}$, $k_{7,8}$, $k_{9,10}$ being the transformer modulus (stoichiometric coefficients) and taking into account the relations of 1-junction, $f_4 = f_8 = f_9 = f_{13}$, we obtain the dynamic equations of the chemical part of the process:

$$dA/dt = F_{inA} - k_{3,4} rV \text{ , } dB/dt = F_{inB} - k_{7,8} rV \text{ (7) } dD/dt = (1/k_{9,10}) rV - F_o \tag{8}$$

where the signification of Bond Graph elements is the following: e_2 is the concentration of reactant A (carbon) [mol/m^3], e_6 is the concentration of reactant B (oxygen) [mol/m^3], e_{11} is the concentration of reaction product D (carbon dioxide) [mol/m^3], F_{inA}, F_{inB} are the reactants input flows [mol/s], F_o is the carbon dioxide outflow rate and r is the reaction rate.

The energetic part of the Bond Graph model from fig. 1 is based on the enthalpy flows and the heat accumulation in the reactor. The energy accumulation in the reactor is modelled using a capacitive element C characterized by the following constitutive equation:

$$e_{15} = \frac{1}{C_{15}} q_{15} = \frac{1}{C_{15}} \int_t (f_{14} + f_{16} + f_{17} - f_{18}) dt \tag{9}$$

with $C_{15} = m_D c_{pD}$ being the parameter of the capacitive element, where m_D is the amount of the reaction product D [kg], and c_{pD} is the specific heat [kJ/kgK].

The input heat flows introduced by the reactants at the initial temperature (298.15K) were modelled by the flow sources Sf_{16} and Sf_{17}. The process output heat flow was also modelled using a source flow element, Sf_{18}. The signification of Bond Graph elements is as follows: e_{15} is the process temperature [K], $f_{16} = m_A c_{pA} (T_i - T_{ref})$, $f_{17} = m_B c_{pB} (T_i - T_{ref})$, and $f_{18} = m_D c_{pD} (T - T_i)$, with $T_i = 298.15$ [K] being the initial temperature and $T_{ref} = 275.15$ [K]. With these notations, the dynamic equation of the thermal part of the process is:

$$m_D c_{pD} \frac{dT}{dt} = m_A c_{pA}(\Delta T) + m_A c_{pA}(\Delta T) + \\ + (\Delta H) k_o e^{-E/RT} C_A C_B V - m_D c_{pD}(T - T_i) \tag{10}$$

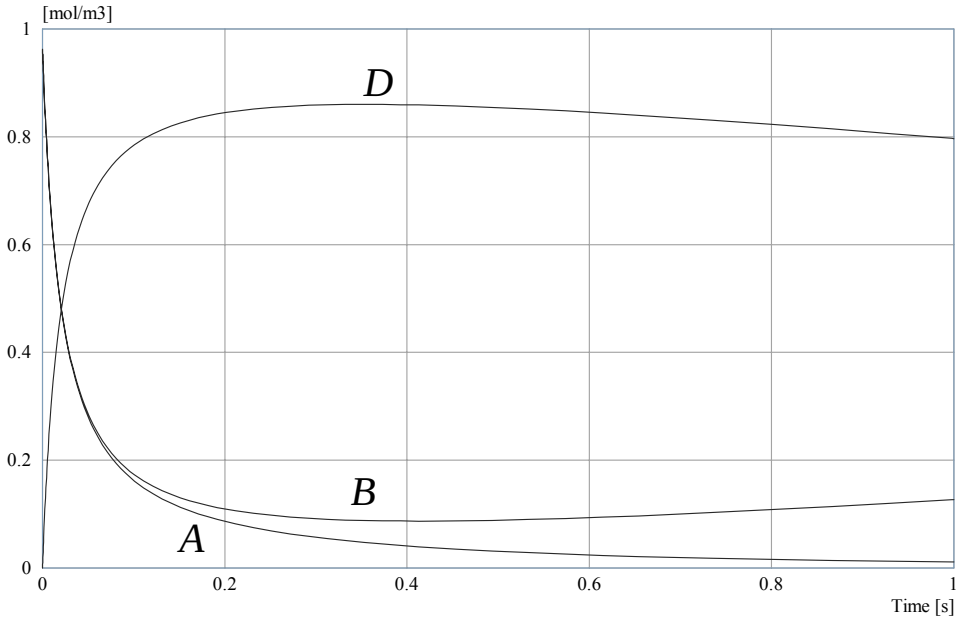

Fig. 2. Time profile of concentrations.

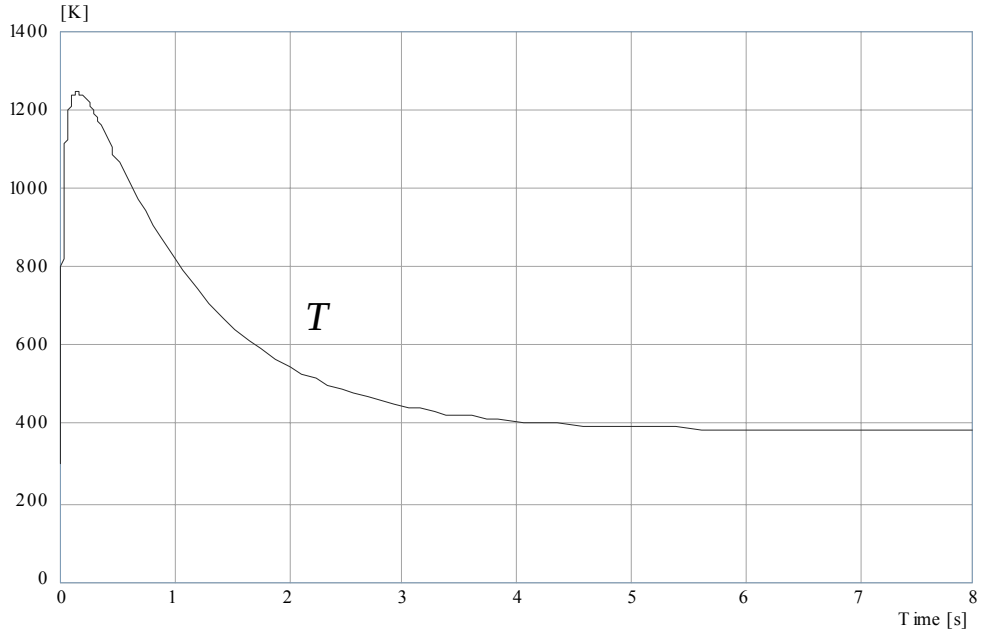

Fig. 3. Time evolution of temperature.

Using 20sim (registered trademark of Controllab Products B.V. Enschede, Netherlands) environment, the Bond Graph model from fig. 1 is implemented. The time profiles of the concentrations and temperature are depicted in fig. 2 and fig. 3. The maximum CO_2 concentration corresponds to the peak in heat released from the reaction (Fig. 3) at a temperature of 1240 [K].

Conclusions

In this paper the Bond Graph modelling was applied to a thermo-chemical process. The work was focused on the combustion process kinetics with respect to reactant and reactor input data. The basic reaction between solid carbon and oxygen was considered to model the combustion solid fuel.

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