

Bond Graph Modeling of an Integrated Biological Wastewater Treatment System

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Extended Abstract

Compared with abstract pure mathematical representation of a system and rough engineering drawings, the concept of bond graphs provide us a unique graphical view based on energy interactions among different domains. Bond graphs sit in the middle between equation sets and schematic block graphs, combining most of the advantages from both. The bond graph approach has already been shown to be effective for modeling, analysis, and design of engineering systems with applications in mechanical translation and rotation, electrical circuits, thermal, hydraulic, magnetic, chemical and other physical domains [1, 2].

In this study, we extend the concepts of bond graphs to the biological domain by defining the basic *effort* and *flow* variables, as free energy of formation, g_i (KJ/mol) and molar flowrate, \dot{n}_i (mol/s), respectively of each species i involved in a reaction. Power/energy (KJ/s) is the product of effort and flow, which are the basic variables that allow systems with diverse energy domain to be treated in a unified manner. Further, since the chemical/biochemical reactions involve stoichiometric relationships, based on the stoichiometry coefficient, v_i , for species i , the biochemical affinity, $v_i g_i$, and electron equivalent flow, \dot{n}_i/v_i [3], are introduced as a conversion of the free energy and molar flowrate.

For each species, a transformer with the stoichiometry coefficient as the *modulus* for that reactant/product represents the conversion of bio-chemical energy between an *inactive* state (the product of free energy and molar flowrate) and an *active* state (bio-chemical affinity and electron equivalent flow). As shown in the lower panel of Figure 1, the difference between the forward (A_f) and reverse (A_r) affinities constitute the true driving force for the chemical reaction to occur.

Applying the newly defined protocols, it is shown how to represent enzyme catalyzed microbe growth, present in wastewater treatment systems and described by Michaelis-Menten, two-step reversible kinetics and Monod kinetics [4, 5] using bond graphs. Figure 2 is a bond graph model of a general Michaelis-Menten equation given by

$$v = \frac{k_p[E]_t[S]}{K_S + [S]} \quad (1)$$

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where $[S]$ is the substrate concentration, $[E_t]$ is the total enzyme concentration, K_S is the Michaelis-Menten constant, v is the overall rate of reaction, and k_p is the dissociation constant.

Similarly Figure 3 represents the bond graph model of a two-step reversible reaction which is a refined representation of Michaelis-Menten kinetics, given by



where P is the product, E is the enzyme, and S is the substrate.

As illustrated in these figures, capacitance (potential energy storage) is used to represent the respective reactants and products, and resistance (energy dissipation) is used to represent reaction kinetics since part of the reaction energy is utilized by the microbes for anabolism and living maintenance or released to the environment directly as heat, a product of temperature (T) and entropy (\dot{S}) [6]. According to the *steady state* assumption [4], it is predictable that all the reactions involved in a two-step reversible kinetics should be represented by two-port resistors showing the combined effects of forward (A_f) and reverse affinity (A_r). Further, in both Figure 2 and 3, the lower loop in the bond graph models represents the dissociation of the enzyme-substrate (ES) complex and release of the free enzyme.

Simulation results using a bond graph model for microbe kinetics described by the two-step reversible reaction given in Equation (2) are shown in Figure 4. In the top panel observe that J_R increases with higher concentrations of the substrate, $[S]$, and lower concentrations of the product, $[P]$, which is determined by the combined effects of forward and reverse affinity. In the lower panel, the dynamics of the two-port resistor based on the effort and flow is illustrated.

Both the choice of Michaelis-Menten kinetics and two-step reversible kinetics are predicated on a microbe population that is non-growing. That is, the total enzyme concentration, $[E]_t$, released by the specific microbe is constant. This assumption is not valid for microbe growth obtained by substrate consumption. To address this issue, Monod kinetics is used [3]. Unlike Michaelis-Menten kinetics, which is derived from first principles, the Monod expressions of the rate of substrate consumption and microbe accumulation are given by,

$$-\frac{d[S]}{dt} = \frac{k[S][X]}{K_S + [S]} \quad (3)$$

$$\frac{d[X]}{dt} = Y \frac{d[S]}{dt} - b[X] \quad (4)$$

In Monod kinetics, the enzyme E is replaced by the microbe biomass X . The minus sign in Equation (3) shows that the substrate is being consumed and hence microbe accumulation is positive. There is a conversion ratio, Y , for substrate consumption to biomass accumulation and in addition, the decay (b) of the microbe.

The bond graph representation of Monod kinetics is shown in Figure 5. When the microbe uses an electron-donor substrate for synthesis, a portion of its electron is initially transferred to the electron acceptor to provide energy for conversion of the other portion of electrons into microbial cells [1]. As shown in Figure 5, a 0-node is used to describe the electron partitioning effect. The reaction inside the dotted area is basically the same as the Michaelis-Menten equation but without considering enzyme increases caused by microbe growth. This part of the reaction is defined as $R^E = R_1^E + R_2^E$, for energy maintenance. The left loop outside the dotted area is for microbe accumulation together with a decay term.

In this work, we demonstrate the concept of bond graphs with the newly defined protocols for enzyme-catalyzed microbe growth to model a coupled bio-reactor system

used for wastewater treatment [7]. The first bio-reactor is a packed bed (PB) reactor that carries out denitrification under anoxic conditions. The second bio-reactor is a tubular (TR) reactor whose feed is the effluent of the first reactor. The TR reactor carries out nitrification at aerobic conditions. The reactions occurring in both reactors can be described by either Monod or Michaelis-Menton kinetics that will be modelled by bond graphs.

Beyond the bio-chemical domain, bond graph modeling will be applied to the hydraulics between the reactors, the mechanics of the peristaltic pump drives and valves supporting the hydraulics, and finally the electronics of the control system. Using the resulting bond graph models of the integrated biological reactor system control and process fault-detection/isolation studies will be investigated [8].

Keywords: Bond graph; Michaelis-Menten equation; Monod kinetics; Modeling; Wastewater treatment; Biological reactor.

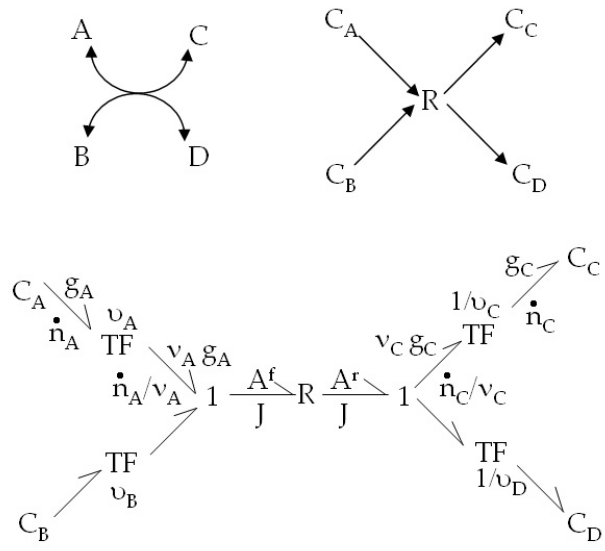


Figure 1: Example : chemical reaction. Upper left panel: multiport dissipator. Upper right panel: 4-port resistor. Lower panel: bond graph.

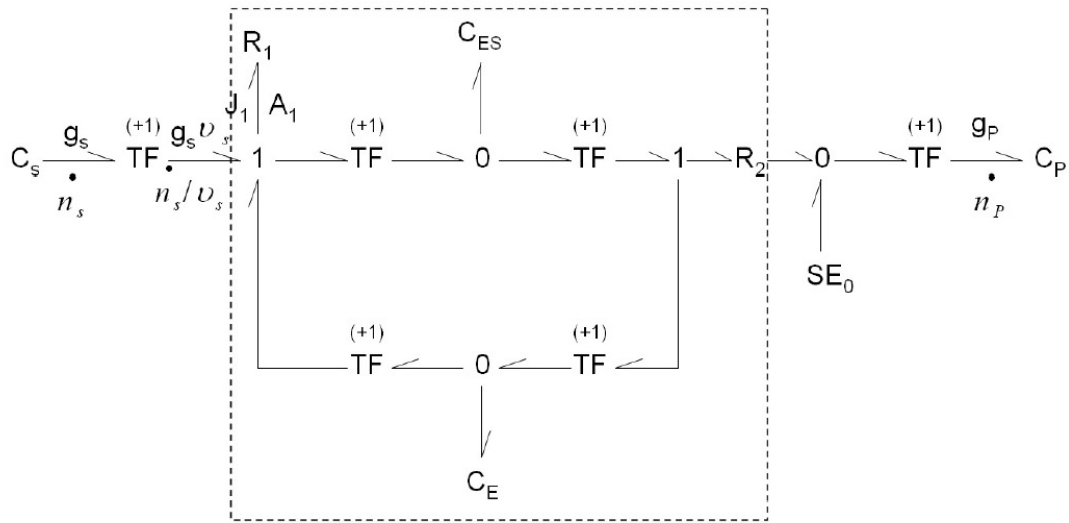


Figure 2: Bond graph model of Michaelis-Menten kinetics.

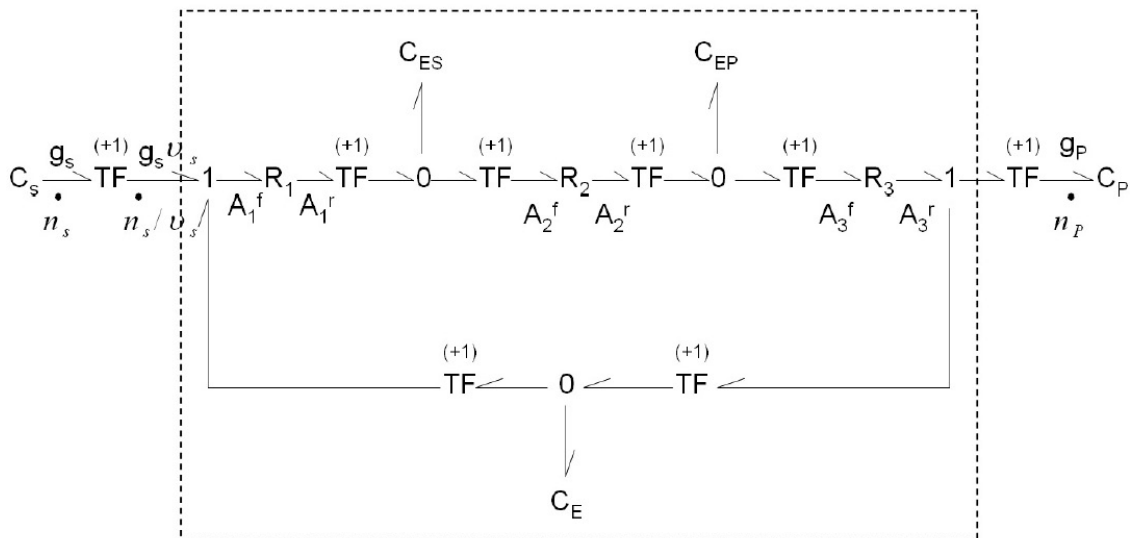


Figure 3: Bond graph model of a two-step reversible reaction.

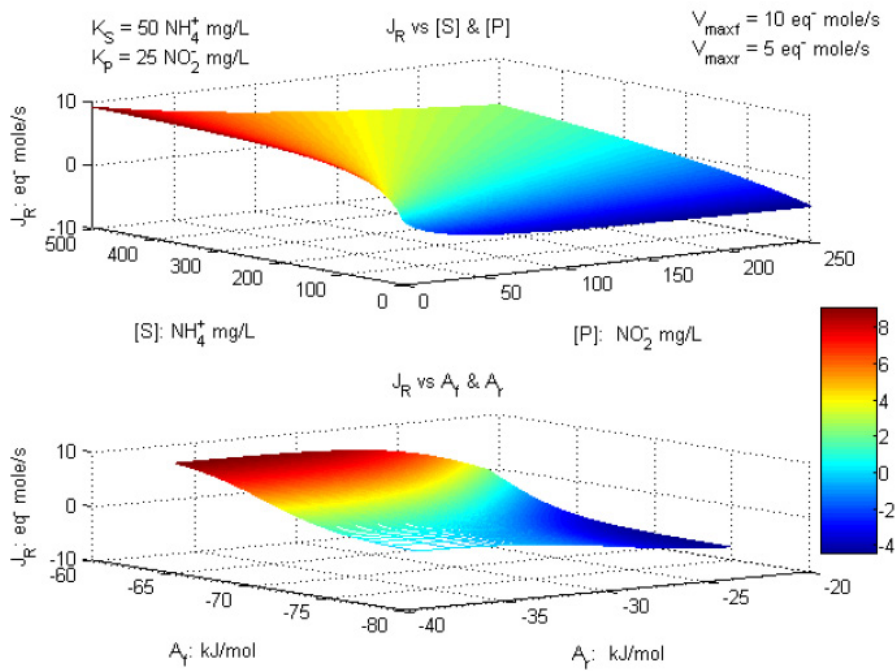


Figure 4: Simulation results for a two-step reversible reaction.

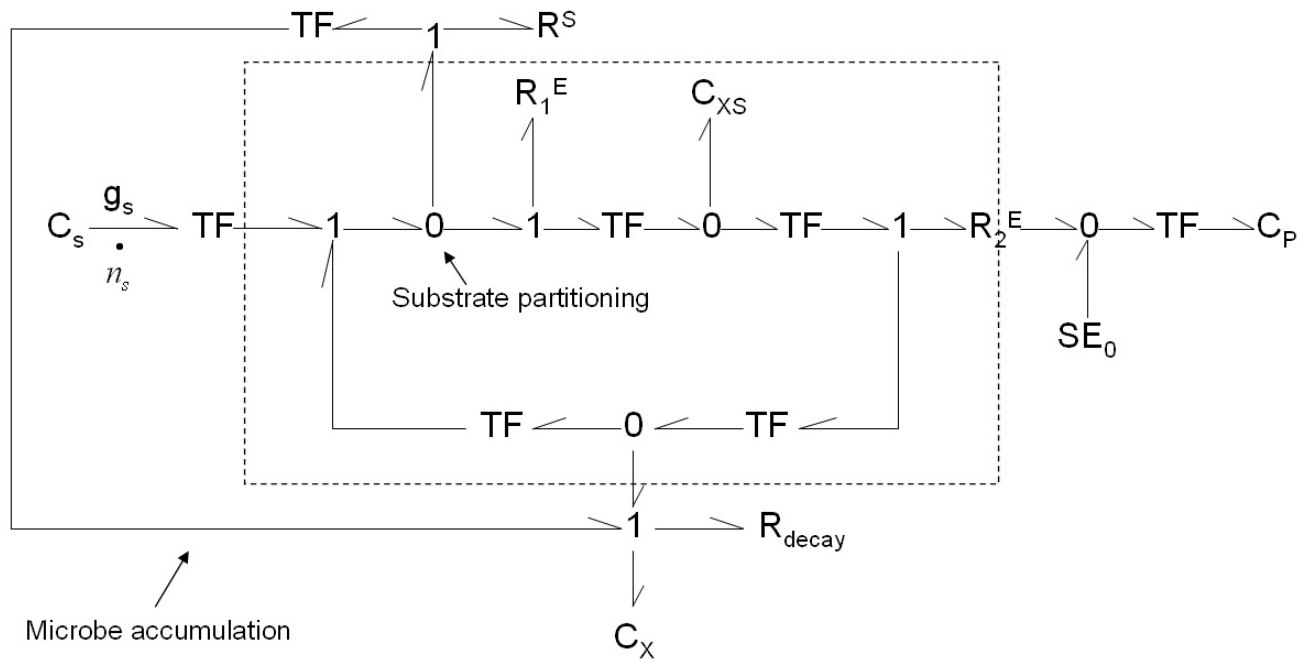


Figure 5: Bond graph model for Monod kinetics

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