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Combined Graph of Pressurized Water Reactor with Autocatalytic Set Approach

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ABSTRACT

Pressurized Water Reactor (PWR) is one of the major systems in nuclear power plant that involved in the generation of electricity. It consists of two major systems namely primary and secondary system. Previously, a graphical representation of the process of operation that occurred in both of the system in the PWR is developed using Autocatalytic Set (ACS) approach. However, analysis obtained through adjacency matrix of each of the ACS graph is inadequate to explain the dynamical process of the operation that involved in the whole system of PWR. Thus, the aim of this paper is to describe the whole system of the PWR by looking at a combination of the ACS graph for the primary and secondary system. Furthermore, Perron-Frobenius eigenvector of adjacency matrix of the combined ACS graph for the whole system of PWR is investigated to explain the dynamical process of the operation that involved in the system. Finally, analysis of the combined ACS graph reveals that the end product of the process of operation in the PWR is in accordance with the previous study.

Keywords: Fuzzy Autocatalytic Set, Adjacency Matrix, Pressurized Water Reactor, Perron-Frobenius Eigenvector

1. Introduction

Nuclear power plant involved many different systems in order to generate electricity. One of the system is Pressurized Water Reactor(PWR) and there are two major systems involved in the PWR namely primary and secondary system Ashaari et al. (2015a) as shown in Figure 1. The primary system transfer heat from the fuel to the steam generator, where the secondary systems begins the conversion of the heat. The steam that is formed from the steam generator is transported to the main turbine generator by the secondary system and this is where the electricity is transformed. The steam is routed to the main condenser after passing through low pressure turbine. Cool water which flowing through the tubes in the condenser allows the steam to condense by removing the excess heat from the steam. Then, the water is pumped back to the steam generator for reuse by USNRC (2011).

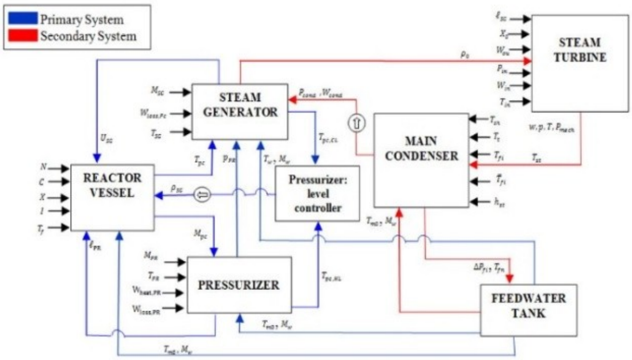

Figure 1: Schematic diagram of a Pressurized Water Reactor(PWR)

The primary and secondary system of PWR exists in one nuclear reactor. All the process of generating electricity which are described above lead to erosion/corrosion in both of the system due to oxygen concentration and PH rate of iron in Wu (1993) and Gedeon (1993). Previously, an Autocatalytic Set (ACS) graph model for both systems is developed Ashaari et al. (2015a). An Autocatalytic Set is defined as a sub graph, each of whose nodes have at least one incoming link from a node belonging to the same sub graph (Jain and Krishna, 1998). As for primary and secondary system in PWR, eight variables that plays vital role in the process are corrosion, moderator, Sulphric acid, Boric acid, Sodium Hydroxide, Chlorides, Nitrogen and fuel. The vertices of the graph correspond to the variables and a directed link from i to vertex j indicates that variable i catalyzes the production of variable j. The network of the interaction between variable in PWR is represented by adjacency matrix. However, this variable is dynamic in nature in which it is wiped out in the process due to it is not functioning and a new network is evolved after certain time t. Thus,graph dynamics represent the dynamical behavior of the variables of the incineration process (Bakar et al. (2013)). Ashaari et al. (2015a) and Ashaari et al. (2015b) had analysed the dynamic of the ACS graph using Perron-Frobenius eigenvector (PFE) of the adjacency matrix which eventually resulted on the evolution of variables on a longer time scale such that the dynamic model provided information of the by-products of the operation process on the PWR (Ashaari et al. (2015b)).

However, the analysis for each ACS graph of primary and secondary system which was made through investigation of its adjacency matrix eventually provided insufficient information to explain the dynamicity of the operation process occurred in the whole system. Therefore, the aim of this paper is to explain the process of operation of the whole system in the PWR by looking at a combination of ACS graph for the primary and secondary system. The vertices and edges of the combined ACS graph represent the variables (chemical compound) and chemical reaction that exist during the process in the whole system of PWR respectively. Subsequently, Perron-Frobenius eigenvector of the adjacency matrix of the combined graph is then investigated to explain the dynamical process of the operation that involved in the system in a form of sequence of depleted variable after certain time t and the result is compared again previous study.

2. An Autocatalytic Set of PWR

The term autocatalytic denotes product or compound used to accelerate a chemical reaction known as catalyst (Bakar et al., 2013). In general, an autocatalytic set is defined as a set of entities or a collection of entities where the word entities can be anything such as people, molecule or object. This is where the graph theory could help in presenting the connection between entities. Graph theory is one of a well-known mathematics that deals with many problems related to structure or network. The application of graph theory not only can be seen in problems related to autocatalytic set but also can be seen in solving location problem (Wan Noor Hayatie et al., 2013, Zati Akmar et al., 2012), railway schedulling problem (Zuraida et al., 2012) and multi-criteria decision making (Noor Hanimah et al., 2008). Further, the perception of an autocatalytic set was presented in the context of relations between compounds which was presented by Jain and Krishna (1998) as follows.

Definition 2.1 Autocatalytic Set (Jain and Krishna, 1998)
An Autocatalytic Set is defined as a sub graph, each of whose nodes have at least one incoming link from a node belonging to the same sub graph.

The illustration of the concept is as below.

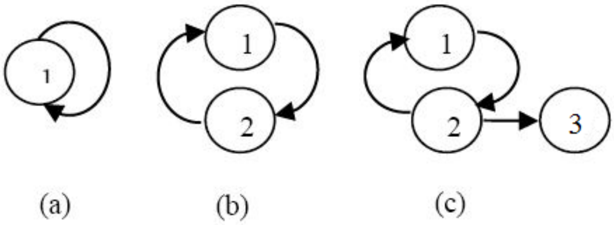

Figure 2: Examples of Autocatalytic Set (ACS)

The following definition of adjacency matrix is used to represent the graph in Figure 2.2.

Definition 2.2: Adjacency matrix (Jain and Krishna, 1998)
An adjacency matrix of a graph $G = G(V, E)$ with n nodes, is an nxn matrix denoted by $C = C_{ij}$ where i, j= 1,2,...,n and C_{ij} equals to unity if there is a link from j to i and zero otherwise.

$$C_{ij} = \begin{cases} 1 & if(v_j, v_i) \in E \\ 0 & if(v_j, v_i) \notin E \end{cases} \tag{1}$$

By using (1), the adjacency matrix for each of the graph in Figure 2 is given as follows.

$$\underset{(a)}{\begin{bmatrix} 1 \end{bmatrix}} \qquad \underset{(b)}{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}} \qquad \underset{(c)}{\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}}$$

Figure 3: Adjacency matrix

The ACS type of graph is also related to irreducible graph as described by the following Definition 2.2, 2.3 and Theorem 1.

Definition 2.3: Irreducible graph by (Harary, 1969)
A graph is termed irreducible if each node in the graph has access to every other node.

Definition 2.4: Irreducible matrix (Harary, 1969).
A matrix A is called irreducible matrix if there exists a positive integer k such that $(A^k)_{ij} > 0$ for every ordered pair of nodes v_i and v_j .

Theorem 1: (Harary, 1969)
Let $A = (a_{ij})$ be a nonnegative matrix. Then the following are equivalent.
a. A is irreducible.
b. For each (i, j), there exists an integer k such that $(A_{ij})^k = (A^k)_{ij} > 0$.
c. A is strongly connected.

The Autocatalytic Set approach has widely been used in modelling of Clinical Waste Incineration Process (CWIP) (Ahmad et al., 2010), Circulating Fluidized Bed boiler (CFB) (Bakar et al., 2013, Ismail et al., 2014) Pressurized Water Reactor (PWR) (Ashaari et al. (2015a); Ashaari et al. (2015b)) and oxy-fuel combustion system (Harish and Bakar, 2017). As for PWR, the ACS graphical model for the primary system is as in Figure 4. Six vertices in the graph represent chemical compound or variable that exist in the primary system as stated in Table 1.

Based on the catalytic relationship between the variables, fifteen edges are identified which are denoted by set E as follows:
$E = \{(v_1, v_3), (v_1, v_2), (v_2, v_1), (v_2, v_3), (v_2, v_4), (v_2, v_5), (v_2, v_6), (v_3, v_2), (v_4, v_3), (v_4, v_1), (v_5, v_2), (v_5, v_3), (v_5, v_4), (v_5, v_6), (v_6, v_3)\}$
Based on the set of vertices and chemical reaction that exist between them, the

Table 1: A set of vertices in the graph of primary system of PWR

Vertices	Variables
v_1	Fuel
v_2	Moderator (H_2O)
v_3	Corrosion
v_4	Boric Acid
v_5	Nitrogen (N_2)
v_6	Chloride (Cl_2)

ACS graph of the primary system is shown below.

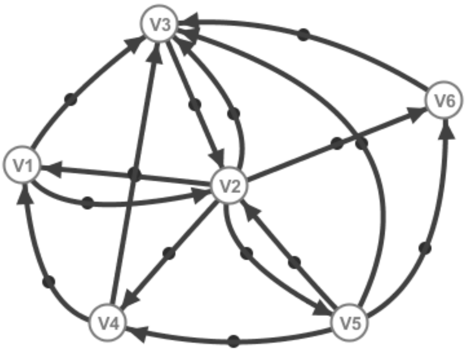

Figure 4: Graph of primary system $G_p = (V, E)$ (Ashaari et al., 2015a,2015b)

Next, for secondary system of PWR, the set of vertices $V = v_1, v_2, v_3, v_4, v_5, v_6, v_7$ namely corrosion, moderator, Sulphuric acid, Boric acid, Sodium Hydroxide, Chlorides and Nitrogen which play an important role in the secondary system of PWR is summarized in Table 2.

Table 2: A set of vertices in the graph of secondary system of PWR

Vertices	Variables
v_1	Corrosion (Co, Zn, Ni, Fe, Zr)
v_2	Moderator (H_2O)
v_3	Sulphuric Acid (H_2SO_4)
v_4	Boric Acid ($B(OH)_3$)
v_5	Sodium Hydroxide (NaOH)
v_6	Chloride (Cl_2)
v_7	Nitrogen (N_2)

Similarly, based on catalytic relationship among the variables,twenty-one edges are constructed and the ACS graph of the secondary system in PWR is shown as follows.

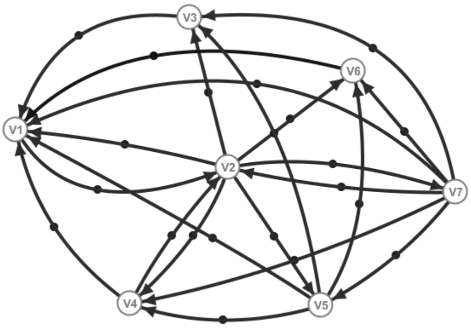

Figure 5: Graph of secondary system $G_p = (V, E)$ (Ashaari et al. (2015c))

3. Combined ACS Graph of PWR

The combined ACS graph, $G_c(V, E)$ is constructed based on the ACS graph of primary and secondary system, $G_p(V, E)$ and $G_s(V, E)$ respectively. This motivates the following definition of combined ACS graph of PWR.

Definition 3.1: Combined ACS Graph of PWR
Let $G_a(V, E)$ and $G_b(V, E)$ be a no-loop ACS graph of two system in PWR and a set of vertices for both graph are $V_a = \{v_{a1}, v_{a2}, ..., v_{an}\}$ and $V_b = \{v_{b1}, v_{b2}, ..., v_{bn}\}$ with set of edges E_a and E_b respectively. A combined graph of PWR, $G_c(V, E)$ is a no-loop ACS graph with combined set of vertices and edges $V_c = \{v_a \cup v_b\}$ and $E_c = \{E_a \cup E_b\}$.

As for chemical compound that exist in both of the system, the vertex representing the compound in both of the graph is then merged into one vertex in the new combined graph. For example, corrosion compound which is represented as v_3 and v_1 in $G_p(V, E)$ and $G_s(V, E)$ respectively is merged as new vertex v_2 in new combined graph $G_c(V, E)$. Similarly, identical reaction that occurred between two vertices that exist in $G_p(V, E)$ and $G_s(V, E)$ is also merged as a new edges in $G_c(V, E)$. For example, (v_2, v_3) is an edges representing reaction between moderator and corrosion in $G_p(V, E)$, while (v_2, v_1) is the reaction between moderator and corrosion in $G_s(V, E)$. Therefore, new links is created and presented as (v_2, v_3) in the combined graph $G_c(V, E)$, where v_2 and v_3 are moderator and corrosion respectively. By following the Definition

3.1 and procedure above, the combined ACS graph of the PWR is presented in Figure 6 and the vertices involved is summarised in Table 3.

Table 3: A set of vertices combined ACS graph of PWR, $G_c(V, E)$

Vertices	**Variables**
v_1	Fuel
v_2	Moderator (H_2O)
v_3	Corrosion Corrosion (Co, Zn, Ni, Fe, Zr)
v_4	Boric Acid ($B(OH)_3$)
v_5	Nitrogen (N_2)
v_6	Chloride Cl_2
v_7	Sulphuric Acid (H_2SO_4)
v_8	Sodium Hydroxide ($NaOH$)

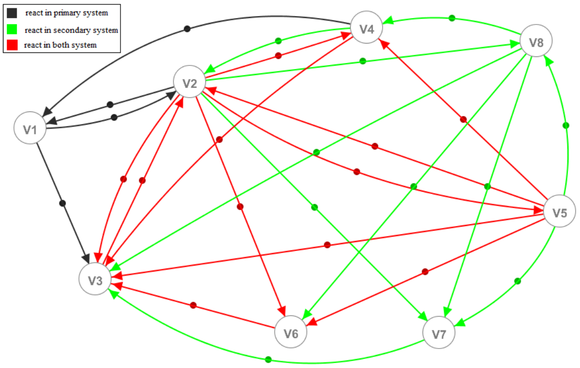

Figure 6: The combined ACS graph of PWR, $G_c(V, E)$

Figure 6 shows the combined graph of $G_p(V, E)$ and $G_s(V, E)$. The graph is an ACS graph since each vertex have at least one incoming link from other vertices in the graph and also a strongly connected graph. Originally, 15 edges exists in the graph $G_p(V, E)$ and 21 edges exist in the graph $G_s(V, E)$ which representing the chemical reaction between any two vertices in the system. Eventually after combining the two graphs, total edges involved in the resulting graph, $G_c(V, E)$ are 25 edges which representing total chemical reactions exist in the whole system of PWR. In the graph $G_c(V, E)$, 4 edges which are symbolised by black colour are chemical reaction involved in the primary system, while 10 edges which are symbolized by green colour are chemical reaction that involved in the secondary system. The balance 11 edges which are represented by red colour are chemical reaction that involved in the both system. Subsequently the study has led to the following proposition.

Proposition 1
Any two-graphs of ACS can be induced to one combined ACS graph.

Proof: Let $G_p(V_p, E_p)$ be an ACS with a set of nodes and a set of edges and $G_s(V_s, E_s)$ be an ACS with a set of V_s nodes and a set of E_s edges. Then the graphs are both irreducible and strongly connected graph which fulfilled Definition 2.2, 2.3 and Theorem 1. Let $V_p = \{x_{p1}, x_{p2}, ..., x_{pi}, ..., x_{pn}\}$, $V_s = \{y_{s1}, y_{s2}, ..., y_{si}, ..., y_{sk}\}$ .Next, if there exist $x_{pi} \in V_p$ and $y_{si} \in V_s$ such that $x_{pi} = y_{si}$ then $V_c = V_p \cup V_s = \{x_{p1}, x_{p2}, ..., x_{pi}\} = \{y_{s1}, y_{s2}, ..., y_{si}\}$. Let $(x_{pi}, x_{pj}) \in E_p$ and $(y_{sc}, y_{sd}) \in E_s$ be an edge correspond to G_p and G respectively. If there exist an e such that $e = (x_{pi}, x_{pj}) = (y_{sc}, y_{sd})$ where $x_{pi} = y_{sc}$ and $x_{pj} = y_{sd}$, then $E_c = E_p \cup E_s = \{(x_{pr}, x_{ps}) \cup (y_{st}, y_{su})\}$. Finally, $G_p(V, E)$ and $G_s(V, E)$ is combined to $G_c(V, E)$.
Immediate case of the Proposition 1 is as follows:

Corollary 1
Autocatalytic Set (ACS) of $G_p(V_p, E_p)$ and $G_s(V_s, E_s)$ of Pressurized Water Reactor (PWR) can be induced to a combine graph $G_c(V_c, E_c)$ where V_c is a set of vertices correspond to the different chemical compound related to the Pressurized Water Reactor (PWR) and E_c is a set of edges correspond to the chemical reaction exist between the compound.

Proof
From Ashaari et al. (2015a) and Ashaari et al. (2015b), the graph of the primary system of PWR is presented as $G_p = (V_p, E_p)$ where $V_p = \{v_1, v_2, ..., v_6\}$ and $E_p = \{(v_i, v_j)\}$ where $i, j = 1, 2, ..., 6$ and the graph of secondary system of PWR is presented as $G_s = (V - s, E_s)$ where $V_s = \{v_1, v_2, ..., v_7\}$ and $E_s = \{(v_i, v_j)\}$ where $i, j = 1, 2, ..., 7$. Both graphs are an ACS graph which fulfilled Definition 2.2, 2.3 and Theorem 1. By using Proposition 1, both $G_p(V_p, E_p)$ and $G_s(V_s, E_s)$ can be induced to a combined graph $G_c(V_c, E_c)$.

Corollary 2
The combined graph $G_c(V_c, E_c)$ of Pressurized Water Reactor (PWR) is an Autocatalytic Set (ACS).

Proof
Let G_c be a combine graph of PWR as stated in the Corollary 1. Suppose for each $i = 1, 2, ..., n, \exists j \neq i, j = 1, 2, ..., i-1, i+1, ..., n, C_{ij} \neq 0$ which means that the i^{th} node must have at least one incoming link, therefore by Definition 2.1(a), the combined graph G_c of PWR is an ACS.

4. Result and Discussion

Next, the adjacency matrix of graph G_c is calculated as follows.

$$C_3 = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

The adjacency matrix C_3 is a nonnegative, square and non-symmetrical matrix. The element is only contains value of 0 and 1 which is non-negative value. Since the graph is strongly connected, then C_3 is irreducible and primitive matrix. All the elements of the diagonal is 0 which shows that there is no self-replicating or no-looping. The largest eigenvalues which is called Perron-Frobenius eigenvalue $\lambda_3(C_3) = 2.932509801646782$ is also calculated and its respective Perron-Frobenius eigenvector (PFE) is determined as

$$\mid X_3(C_3) \mid = \begin{bmatrix} 0.251203103506086 \\ 0.456634807494564 \\ 0.652147515595991 \\ 0.280020755741124 \\ 0.155714673907701 \\ 0.280020755741124 \\ 0.280020755741124 \\ 0.208814129473120 \end{bmatrix}$$

The value in the PFE element can be used to represent the degree of significant for the chemical compound/variables to be exists in the process for the next time interval (Bakar et al. (2013)). The larger the value of the element in PFE, the stronger the variable (chemical compound) to be remain in the system. Similarly, the lower the value of the PFE element means that the variables are eventually not significant and eventually depleted from the system. This is may be due to the amount of rate of concentration of the compound that is small enough to make any impact to the next process. As for the above PFE, Table 6 shows the sequence of the depleted variables and the variables that is left at the end of the system using adjacency matrix for the combined ACS graph of PWR, $G_c = (V_c, E_c)$ as compared to G_p and G_s.

Table 4: Sequence of the depleted variables for combined graph,$G_c(V, E)$

	Adjacency matrix		
	$G_p(V, E)$	$G_s(V, E)$	Combined ACS, $G_c(V, E)$
Sequence of depleted variables	Nitrogen(N_2), Chloride (Cl_2), Boric Acid ($B(OH_3)$), Fuel	Nitrogen(N_2). Sodium Hydroxide (NaOH), Chlorides (Cl_2), Boric Acid ($B(OH_3)$), Sulphuric Acid (H_2SO_4)	Nitrogen(N_2), Sodium Hydroxide (NaOH), Sulphuric Acid (H_2SO_4), Chlorides (Cl_2), Boric Acid ($B(OH_3)$), Fuel
Variables that is left when system shut down	Moderator (H_2O) Corrosion (Co,Zn, Ni,Fe,Zr)	Moderator (H_2O) Corrosion (Co,Zn, Ni,Fe,Zr)	Moderator (H_2O) Corrosion (Co,Zn, Ni,Fe,Zr)

Based on Table 4, Nitrogen is the first chemical compound that is depleted for primary, secondary and the combined system using adjacency matrix. Nitrogen is depleted first due to the activation of Oxygen, which resulting the formation of Nitrogen-16 Ashaari et al. (2015a). Chlorides is depleted at time t_1, t_2 and t_3 in primary, secondary and combined system respectively due to presence of nitrogen (Ashaari et al., 2015b). Next, Sodium hydroxide is depleted. Sodium Hydroxide is a medium of heat transfer and it is depleted due to no heat transmission occur in the process of PWR. Boric acid is depleted at time t_4 in combined system due to the excessive reaction in the PWR. Then, the fuel compound is depleted, and this indicates that the fuel compound is completely used in operation of PWR. From this table, it indicates that the chemical compound depleted at different time t, however, the variables that is left when the system is shut down for the three systems are the same, which is Moderator and Corrosion. The moderator is needed to exist until the end of the operation to prevent the system from overheating Ashaari et al. (2015a).While, due to chemical reaction during long-term operation in the PWR system, the corrosion exists. The corrosion's product and moderator exist till the end of the process which is confirmed by Murray (2009), Ashaari et al. (2015a) and Ashaari et al. (2015b).

5. Conclusion

Combined ACS graph of primary and secondary system of PWR is successfully presented. The procedure and the development of the graph are explained. The dynamics of the process involved in the PWR which is analysed through Perron-Frobenius eigenvector of the adjacency matrix is presented and the result is compared with the previous study indicates the similar result but with better explanation in term of sequence of depleted variables involved in the PWR. The combined graph $G_c(V,E)$ could serve as one graph representation for the PWR as it not only could explain the process involved in the whole system of PWR but could also explain the dynamic nature of the process involved in the whole system. Besides, analysis of the dynamic of the operation process of the whole system could be less time consuming since only one combined graph is involved.

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