Dynamic Graph Model of Evaporation Process in a Boiler System

H. Noor Ainy, A. Tahir& I. Razidah

***Abstract*—**Traditionally, research on graph theory focused on studying the properties of static graphs. However, almost all real networks are dynamic and large in size. Quite recently, study on evolution of variables or processes in the network have led to the integration of the concept of Autocatalytic set (ACS) and Graph theory. Thus, this paper aims to develop the dynamic graph model of an evaporation process in a Boiler system whereby seventeen variables are identified to represent the nodes. Thirty six links which are based on the catalytic relationship among the nodes represent the edges. Based on the concept of ACS, new properties of the graph are revealed. These properties indicate some initial findings that will lead to the further exploration in terms of Fuzzy Graph.

***Keywords*—**Combustion process, Corrosion, Water treatment, Perron-Frobenius eigenvector.

I. Introduction

GRAPH theory provides a mathematical modeling for studying interconnection among elements in natural and man-made systems. Traditionally, research on graph theory focused on studying static graphs. Directed graph is widely used to interpret the interconnection structure underlying the dynamics of the interacting subsystems or variables involve in the process. Recently, study on evolution of variables or processes have become the most active areas of research [1] – [3].

The concept of autocatalysis comes from chemistry. An Autocatalytic Set (ACS) is a set of reactions whose product catalyzes one another. In term of graph theoretic approach, ACS is a subgraph each of the nodes has one incoming link from a node belonging to the same subgraph [4]. Applications of this concept are explored in modeling the clinical waste incineration process and combustion process in a Circulating Fluidized Bed Boiler [2,10]. There are two main processes involve in a typical oxy-fuel combustion boiler system namely, combustion and evaporation process. In power generation plant, steam is used to generate electricity. Steam is produced by evaporation process in the boiler system which involves complex interactions of chemical substances that exist during the process. Since these chemical substances will undergo evolution process, the evaporation process can be represented as the dynamic graph by integrating the concept of Autocatalytic set.

The evaporation process in the boiler system is described in the next section, which is followed by some discussion on the concept of ACS utilized in developing the dynamic graph model. Next, some properties related to the dynamic graph model are revealed.

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II. Evaporation process in Boiler System

Since corrosion is the main cause of reduced reliability in steam generating systems, proper water treatment to the feedwater system is essential in order to protect tubes and heaters in the boiler system against corrosion. Regardless of feedwater design, the major problems are similar for all types of system [5]. Based on Fig. 1 which is adapted from [3], the feedwater is supplied to the drum where the water is evaporated. The furnace is used to increase the water temperature and eventually to cause evaporation. Thus, circulation of water, steam, and water and steam mixture take place in the drum where steam generated in the drum flows to other systems in the boiler.

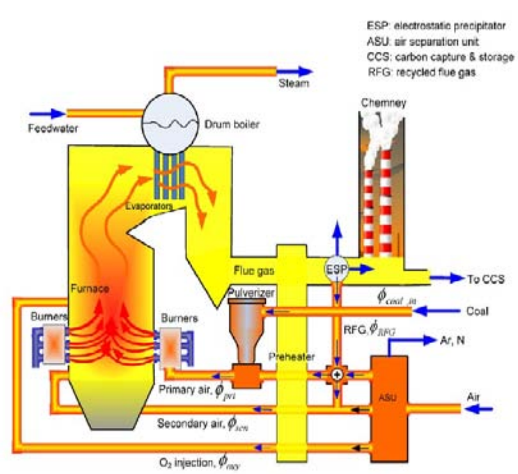


Fig. 1 Evaporation process in oxy- combustion Boiler

The steam drum is the entry point for feedwater and internal chemical treatment. The dynamic graph of evaporation process in drum system depends on chemical reactions in the feedwater-drum system [5].

III. THE AUTOCATALYTIC SET

The concept of Autocatalytic set (ACS) was formally introduced in 1971 by Kauffman, Eigen and Rossler as a set of catalytically interacting molecules. Later, Jain and Krishna [4] had integrated ACS in terms of graph theoretical concept and formalized as follows:

Definition 1: Autocatalytic Set
An autocatalytic set is a subgraph, each of whose nodes has at least one incoming link from a node belonging to the same subgraph.

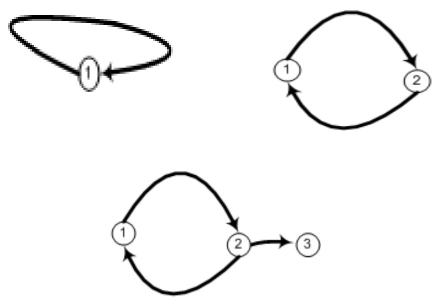


Fig. 2 Examples of ACS

Some examples of ACS are shown in Fig. 2, where a node in a directed graph represents a molecular species and a link from *j* to *i* indicates that *j* is a catalyst for *i*.

A graph with *s* nodes is completely specified by a matrix of order *s*, $A=(a_{ij})$ called the adjacency matrix of the graph. The graph is transformed to a square adjacency matrix, *A* by using definition of adjacency matrix given in [4] where

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

By using (1), the adjacency matrices of the graphs in Fig. 2 are represented as follows.

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

Here, the adjacency matrix in (1) is the transpose of usual adjacency matrix as defined by [10]. This convection had been adopted by [1, 2] in their works as it is convenient and representative in the context of the dynamical systems.

IV. DYNAMIC GRAPH MODEL OF EVAPORATION PROCESS

A digraph *G* is formally defined by $G=(V,E)$ where *V* is the set of vertices and *E* is the set of arcs or edges; each being a pair of distinct vertices. The set of vertices, *V* which signify chemical substances or variables that play the vital role in the water treatment and evaporation process in feedwater-drum system are identified as Pollution(v_1), Scavengers(v_2), Water(v_3),Metal oxide(v_4), Sodium sulfite(v_5),Oxygen(v_6),Nitrogen(v_7),Sodium hydroxide(v_8), Sulfur dioxide (v_9), Hydrogen sulfide(v_{10}), Hydrocloric acid(v_{11}), Sodium chloride (v_{12}), Hydrogen(v_{13}), Copper oxide(v_{14}), Silicon dioxide(v_{15}), Carbon dioxide(v_{16}) and Sulfuric acid(v_{17}). Pollution (v_1) represents the corrosion deposits and gases that is transported to the outside of the feedwater-drum system whereas scavengers (v_2) refers to the chemical treatment which is added to control corrosion. Based on the chemical reactions in [5]–[9], thirty six edges, *E* which represent the links between variables in the water treatment process due to their catalytic relationship are identified. As an example, the link (v_2,v_4) is based on the chemical reaction, $N_2H_4+6FeO_3\rightarrow 4Fe_3O_4+N_2+2H_2O$ [6]. This means that scavengers (v_2) namely hydrazine(N_2H_4) catalyzes the formation of metal oxide,(Fe_3O_4) (v_4)as shown in Fig. 3. Metal oxides prevent contact between metal and oxidizing ions in the boiler tube.

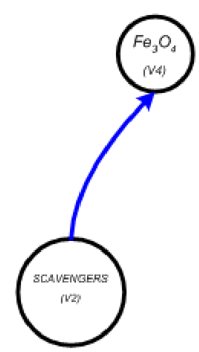


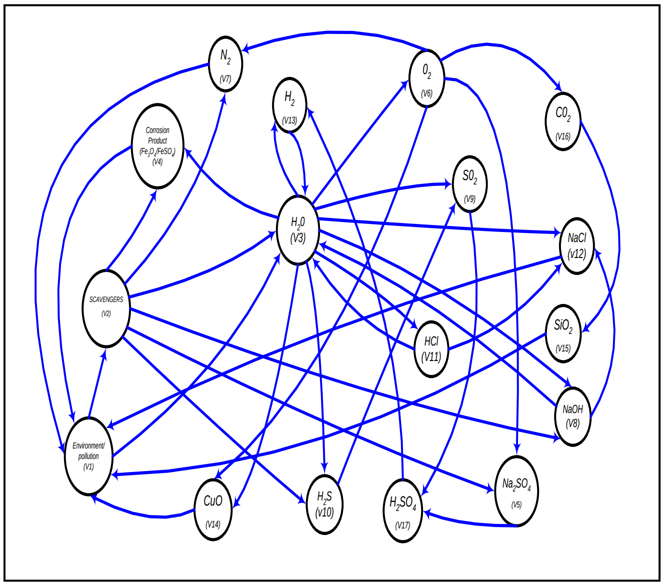
Fig. 3 The link, (v_2,v_4)

Thus, the complete set of *E* is as follows

$$\begin{aligned}E=\{&(v_1,v_2),(v_1,v_3),(v_2,v_3),(v_2,v_4),(v_2,v_5),(v_2,v_7),(v_2,v_8),(v_2,v_{10}),\\&(v_3,v_4),(v_3,v_6),(v_3,v_8),(v_3,v_9),(v_3,v_{10}),(v_3,v_{11}),(v_3,v_{12}),(v_3,v_{13}),\\&(v_3,v_{14}),(v_4,v_1),(v_5,v_{17}),(v_6,v_5),(v_6,v_7),(v_6,v_{14}),(v_6,v_{16}),(v_7,v_1),\\&(v_8,v_3),(v_8,v_{12}),(v_9,v_{17}),(v_{10},v_9),(v_{11},v_3),(v_{11},v_{12}),(v_{12},v_1),(v_{13},v_3),\\&(v_{14},v_1),(v_{15},v_1),(v_{16},v_{15}),(v_{17},v_{11})\}\end{aligned}$$

Hence, dynamic graph model of the evaporation process denoted as $G_S(V,E)$ is shown in Fig. 4.

Fig. 4 Dynamic graph model of the evaporation process $G_S(V,E)$



Based on the definition of an Autocatalytic set given in previous section and the description on the catalytic relationship between the chemical substances have provided a proof by construction for the following proposition.

Proposition1: The graph, $G_S(V,E)$ is an Autocatalytic set.

This proposition has inspired to explore further features of the dynamic graph model.

V. RELATED PROPERTIES OF THE GRAPH, $G_S(V,E)$

A. *Irreducible graph*

The first property to explore is to determine whether the graph is reducible or irreducible. A graph is said to be irreducible if each node in the graph has access to every other node. In addition, an irreducible graph is an ACS [4]. Therefore, the graph, $G_S(V,E)$ as shown in Fig. 4 is an ACS, hence, it is an irreducible graph.

B. *Adjacency Matrix*

The graph, $G_S(V,E)$ represents the network of chemical interaction in the evaporation process where the chemical substances or variables are represented as nodes and directed link from node *j* to node *i* indicates that variable *j* catalyzes the production of variable *i*. Hence, the corresponding adjacency matrix, *A* of the graph, G_S is a nonnegative matrix which is irreducible and primitive [2]. The special feature of the matrix of the graph, G_S is that every row must contain at least one non–zero element. It is also shown that all the elements of principle diagonal of the matrix are zero. This shows that there is no self-replicating of any of variable within the system.

C. *Relation of an ACS to Perron-Frobenius eigenvector*

The ACS is a useful graph-theoretic concept which can be related to the Perron-Frobenius eigenvector[11]. The Perron-Frobenius eigenvector (PFE) is an indicator of the existence of ACS in a graph. The relation of its corresponding adjacency matrix, *A* to Perron-Frobenious Theorem [11] showed that the largest value known as Perron-Frobenious eigenvalues is $\lambda_1 \geq 1$ for graph $G_S(V,E)$ and its corresponding eigenvector (PFE) is denoted as X_S.

$$A=\begin{bmatrix}
0&1&1&0&0&0&0&0&0&0&0&0&0&0&1&0&0\\
0&0&1&1&1&0&1&1&0&1&0&0&0&0&0&0&0\\
0&0&0&1&0&1&0&1&1&1&1&1&1&1&0&0&0\\
1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\
0&0&0&0&1&0&1&0&1&0&0&0&0&1&0&1&0\\
1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&0&0&0&0&0&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\
0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0\\
0&0&1&0&0&0&0&0&0&0&1&0&0&0&0&0&0\\
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1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0
\end{bmatrix}, \quad X_S=\begin{bmatrix}
0.3846\\0.1496\\0.4647\\0.2388\\0.1284\\0.1807\\0.1284\\0.2388\\0.2735\\0.2388\\0.1807\\0.3438\\0.2414\\0.2509\\0.0273\\0.0703\\0.1563
\end{bmatrix}$$

Since all elements of PFE are non-zero, it can be deduced that the subgraph of the PFE is the entire graph $G_S(V,E)$ which further confirmed that the graph, $G_S(V,E)$ is an ACS. Thus PFE can be considered to be an indicator for the existence of ACS in the graph.

VI. CONCLUSION

Dynamic graph model of an evaporation process in a Boiler system is developed with Autocatalytic set as its main features. By considering the chemical reactions in the water treatment and evaporation process, seventeen chemical substances are identified to represent the nodes and thirty-six links to represent the edges of the graphical model. In addition, some properties of the graphical model related to adjacency matrix and Perron-Frobenius Theorem are presented. Thus, the relationship of Autocatalytic set and Perron-Frobenius eigenvector has provided a better understanding of the graph representing the evaporation process in the boiler system. It is anticipated that the approach adopted in this work will lead to further research by considering uncertainty or fuzziness in modeling complex dynamical systems.

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