

Modeling a clinical incineration process using fuzzy autocatalytic set

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Abstract In this paper we have investigated and explored the realm of fuzzy graph in its relation to autocatalytic sets. A new concept namely fuzzy autocatalytic set have been defined. This relation has produced some results in the forms of theorems which have been proven. A clinical waste incineration process has been modeled using this new concept indicates to be more accurate than using crisp graph.

Keywords Fuzzy graph · Fuzzy autocatalytic set · Incineration process · Chemical engineering

1 Introduction

Ever since Zadeh [20] introduced the idea of fuzzy set theory by utilising the concept of grade membership, numerous researchers have been concerned with the properties and applications of fuzzy sets [4, 8, 9, 11, 17]. This is due to the fact that certain aspects of reality such as complexity and ill-defined situations always escape most crisp mathematical models. Thus the crisp models usually inadequate in describing the whole process of the systems.

Fuzzy graph was another extension of fuzzy theory's application in its relation to graph theory. Rosenfeld [14] has defined fuzzy graph in which he has considered fuzzy graph to consist both fuzzy set for vertices as well as for the edges given as follows:

Definition 1.1 Fuzzy graph $G = (\sigma, \mu)$ is a pair of functions $\sigma : S \rightarrow [0, 1]$ and $\mu : S \times S \rightarrow [0, 1] \quad \forall x, y \in S$, we have $\mu(x, y) \leq \sigma(x) \wedge \sigma(y)$.

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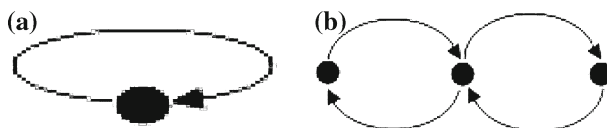


Fig. 1 **a** A 1-cycle, the simplest ACS. **b** An irreducible graph but not cycle

Yeh and Bang [19] also coined a special case of graph fuzziness where only the edges are fuzzy and the vertices remain as a crisp set. Blue et al. [1,2] further generalized the catalog of various types of fuzziness possible in graphs, which they called taxonomy of fuzzy graphs. These graphs can be classified into 5 types as follows:

Type 1: Fuzzy Set of Graphs

Type 2: Crisp Vertex Set and Fuzzy Edges

Type 3: Crisp Vertices and Edges with Fuzzy Connectivity

Type 4: Fuzzy Vertex Set and Crisp Edge Set

Type 5: Crisp Graph with Fuzzy Weight.

Even though these classifications cover the whole range of possible ‘fuzziness’ of a graph, however, a real working model of a system remains illusive. In the following sections we will present how these graphs are related to autocatalytic set proposed by Jain and Krishna [6] and how it help to model an incineration process.

2 Fuzzy autocatalytic set

The concept of autocatalytic set (ACS) was first introduced in the context of catalytically interacting molecules, [7,13]. However, Jain and Krishna [6] have formalized the autocatalytic set in terms of graph theoretical concept (see Fig. 1) as follows:

Definition 2.1 An autocatalytic set is a subgraph, each of whose nodes has at least one incoming link from a node belonging to the same subgraph (see Fig. 1).

The main idea for the definition of fuzzy autocatalytic set (FACS) is the merger of fuzzy graph concept as discussed in Sect. 1, in particular Type 3 and the concept of an autocatalytic set. The formal definition is given as follows:

Definition 2.2 Fuzzy Autocatalytic Set (FACS) is a subgraph each of whose nodes has at least one incoming link with membership value $\mu(e_i) \in (0, 1]$, $\forall e_i \in E$.

The membership values for fuzzy edge connectivity for fuzzy graph are in the interval $(0, 1]$. These values constitute the entries of the adjacency matrix for fuzzy graph. With this difference in values to the adjacency matrix of fuzzy graph as compared to the value of 0 and 1 in the adjacency matrix of crisp graph would result in the difference of their algebraic structure. Such differences are presented in the following theorems.

Theorem 2.1 *If G is an FACS with adjacency matrix*

$$C_G = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad (2.1)$$

and for each $\alpha = 1, 2, \dots, n$, there exist $\beta \neq \alpha$, $\beta = 1, 2, \dots, \alpha - 1, \alpha + 1, \dots, n$ such that $a_{\alpha\beta} \neq 0$, then $a_{ij} a_{si} a_{ts} \cdots a_{pl} a_{jp}$ is a cycle.

Proof Suppose G is an FACS with adjacency matrix C_G as above. Next consider the sequence of non-zero entries of C_G as $a_{ij} a_{si} a_{ts} \cdots a_{pl} a_{jp}$. Look

a_{ij} indicates there exist a link from j to i ,
 a_{si} indicates there exist a link from i to s ,
 a_{ts} indicates there exist a link from s to t ,
 \vdots
 a_{pl} indicates there exist a link from l to p and
 a_{jp} indicates there exist a link from p to j .

Since all links are connected and the path starts and ends at the same point (vertex), therefore the sequence in the form of

$a_{ij} a_{si} a_{ts} \cdots a_{pl} a_{jp}$ must be a cycle. \square

FACS can be linked with Perron-Frobenius Theorem in particular its relation to the PFEs. This resulted in the following theorem.

Theorem 2.2 *If a graph is an FACS, then $\lambda_1 > 0$.*

Proof Suppose G_F is an FACS, therefore G_F must contain a cycle by Theorem 2.1. There exist a node that has at least one path to itself of length n with some fuzzy connectivity such that $(C^k)_{ii} > 0$ for $k \in \mathbb{Z}^+$. We know that the summation of Eigen values is its trace; $\sum_{i=1}^s (C_{ii}) = \sum_{i=1}^s \lambda_i$, [10], similarly

$$\sum_{i=1}^s (C^k)_{ii} = \sum_{i=1}^s (\lambda_i^k). \quad (2.2)$$

Using the fact $(C^k)_{ii} > 0$ and Eq. 2.2, therefore

$$\sum_{i=1}^s (\lambda_i^k) > 0 \quad (2.3)$$

and from Eq. 2.3,

$$\left| \sum_{i=1}^s (\lambda_i^k) \right| > 0. \quad (2.4)$$

Now, using the triangle inequality, [18]

$$\sum_{i=1}^s |(\lambda_i^k)| \geq \left| \sum_{i=1}^s (\lambda_i^k) \right| \quad (2.5)$$

$$\text{Using Eq. 2.3, 2.4 and 2.5, therefore } \exists \lambda_i^k \text{ for some } i \left| \lambda_i^k \right| > 0. \quad (2.6)$$

Consequently, $\lambda_1 = |\lambda_i^k|$ is the dominant eigenvalue with the largest modulus greater than zero. \square

3 An incineration process

Clinical or medical waste is defined as a waste which consists wholly or partly of human and animal tissue, blood or any other body fluids, excretions, drugs or pharmaceutical products, swabs or dressings, or syringes, needles, or sharp instruments that is hazardous to any person coming into contact with it. It also includes waste arising from medical, dental, veterinary, pharmaceutical or similar practice, investigation, treatment, care, teaching, or research, or collection of blood for transfusion that may cause infection to any person coming into contact with it.

Incineration is known to be the best available option for treating such waste particularly the pathological related waste. It appears to be the ideal solution to clinical waste management mainly because it has the capability of destroying hazardous components of a waste and of reducing a waste's volume by leaving only ash to dispose of. Although it is a preferred method of disposal, the air impurities associated with the burning of the waste is a major concern to the public [12]. This includes the product of incomplete combustion consisting of organic compounds which are toxic even at extremely low concentrations. Polychlorinated dibenzo-p-dioxin (referred to as dioxin) and polychlorinated dibenzo-furans (or furan) are two such toxic combustion products.

Since there is no fundamentally based mathematical model to explain the underlying principles involving the incineration process and operational control of the incinerator, a study was carried out to model the process using graph. A regional clinical waste incinerator facility in Malacca (schematic diagram given in Fig. 2), owned by Pantai Medivest Sdn Bhd known formerly as Tongkah Medivest Sdn Bhd was selected and modeled in the research [16]. It is estimated that 200 metric tons of clinical waste being generated throughout the southern region of Peninsular Malaysia every month from hospitals and clinics and this waste is being catered for by this facility.

The initial graph modeled in the study with the components of the incinerator denoted as vertices and the input-output variables as the edges [15] is seen to be static in nature (Fig. 3) and not much of its properties can be studied. Therefore, a dynamic model of the incineration process is sought for.

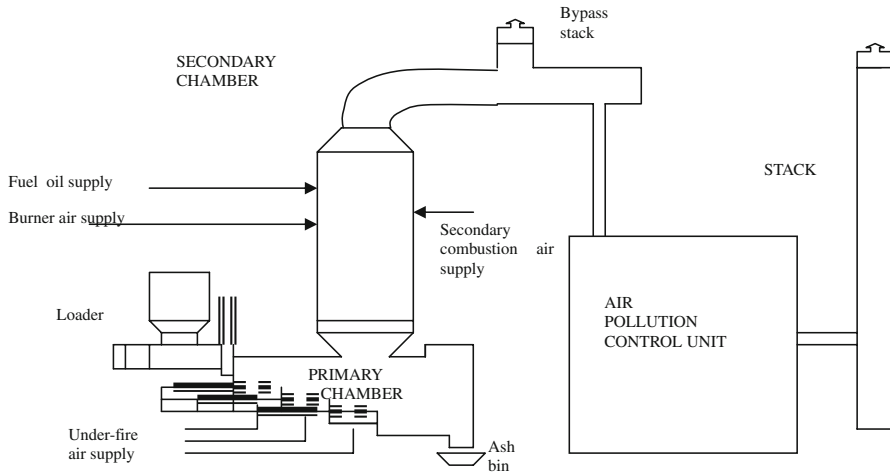


Fig. 2 The schematic diagram of a clinical waste incinerator

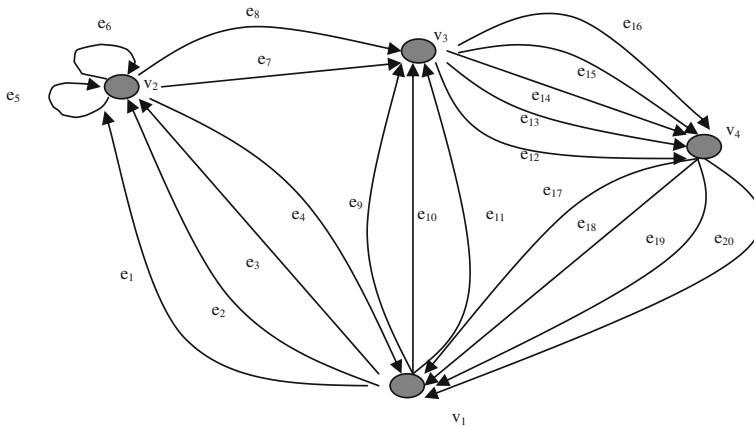


Fig. 3 Graph showing the association between input–output variables and different components of the incineration process

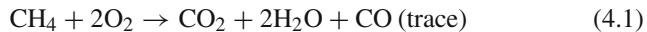
- v_1 : Environment
- v_2 : Primary combustion chamber (PCC)
- v_3 : Secondary combustion chamber (SCC)
- v_4 : Air pollution control unit (PCU)
- e_1 : Wood
- e_2 : Clinical waste
- e_3 : Underfire Air—Air 1
- e_4 : Ash
- e_5 : Temperature (Zone 1 and 2)—Temp1
- e_6 : Temperature (Zone 3)—Temp2
- e_7 : The product of combustion

- e₈: Temperature at the inlet of the secondary chamber—Temp3
- e₉: Fuel
- e₁₀: Burner air supply—Air2
- e₁₁: Secondary combustion air supply—Air3
- e₁₂: Temperature at the outlet of the secondary chamber to the PCU—Temp4
- e₁₃: Carbon monoxide
- e₁₄: Carbon dioxide
- e₁₅: Oxygen
- e₁₆: Pollutants
- e₁₇: Oxygen
- e₁₈: Carbon monoxide
- e₁₉: Carbon dioxide
- e₂₀: Pollutants

4 A dynamic model

The four components of the incinerator plant were discarded (see Fig. 3) from graph and the emphasis of the study was to investigate the role played by the variables in the incineration process [16]. In this regard, the process was assumed to be taking place in one compartment; the incinerator. This led to the development of the dynamic graph G_d . $V = \{v_1, v_2, v_3, v_4, v_5, v_6\}$ is the set of vertices represent six variables that play vital roles in the clinical waste incineration process, namely waste, fuel, oxygen, carbon dioxide, carbon monoxide and other gases including water, respectively. Fifteen edges of E represent the links of the variables in the process due to their catalytic relationship [16] given as follows.

- (v_1, v_2) : *Waste particle interact with fuel in the chamber to initiate and aggravate the combustion process. Apparently, besides diesel, waste is also considered as part of fuel for the process.*
- (v_1, v_3) : *One of the products of combustion based on chemical composition of waste specified by Green [5] is O_2 . This means that waste is contributing a certain amount of O_2 to the chamber. In fact, the initial amount of O_2 in the chamber taken as the concentration dynamics of this variable relates to this interaction.*
- (v_1, v_4) : *CO_2 is the product of combustion waste. Consequently, waste catalyzed the production of CO_2 .*
- (v_1, v_5) : *CO is also the product of combustion of waste. This gas is produced as a result of an insufficient amount of O_2 in the chamber.*
- (v_1, v_6) : *H_2O and Pollutants are the products of combustion of waste. Therefore, waste catalyzed the production of these variables.*
- (v_2, v_4) : *In the waste and fuels normally encountered, the major constituents include carbon and hydrogen. The fuel (diesel) used in the chamber must also contribute to the production of CO_2 .*
- (v_2, v_5) : *In the case where O_2 is insufficient, there is trace of production of CO in the chamber. Bruner [3] explained the production of CO by the following equation.*



(v_2, v_5) : Equation (4.1) indicates that water is catalyzed by fuel.

(v_3, v_1) : 11% of waste constitutes of O_2 [5]. O_2 is part of the waste especially at its initial stage in the chamber.

(v_3, v_4) : O_2 catalyzes the formation of CO_2 .

(v_3, v_5) : The equation



shows that O_2 is the variable that motivates the formation of CO . CO is produced where insufficient oxygen is provided to completely combust a fuel.

(v_3, v_6) : O_2 and other molecules presence in waste and also fuel such as in Eq. 4.1.

(v_4, v_6) : CO_2 is a stable gas. But there are circumstances whereby, it will react with water vapor in the chamber to produce carbonic acid which we classified as v_6 .

(v_5, v_4) : CO can react with O_2 to form CO_2 . The reaction took place when excess amount of O_2 is in the chamber. It is the intermediary reaction between carbon and oxygen to form CO_2 and if CO was formed instead, it will automatically react or mix with more oxygen to form CO_2 .

(v_6, v_1) : About 23% of waste constitutes of water (H_2O) as shown by Green [5].

By the definition of autocatalytic set given in Sect. 2.1 and catalytic relationship described earlier, we can have the following theorem by construction.

Theorem 4.1 The graph $G_d(V, E)$ is an autocatalytic set.

5 A fuzzy graph type 3

Eventhough Rosenfeld [14] and shortly Yeh and Band [19] have given the definitions of a fuzzy graph, however, we can formalized five types of fuzziness possible in graphs as described by Blue et al. [1,2] in the following.

Definition 5.1 Fuzzy graph is a graph G_F satisfying one of the fuzziness (G_F^i of the i^{th} type) or any of its combination:

- i. $G_F^1 = \{G_{1F}, G_{2F}, G_{3F}, \dots, G_{nF}\}$ where fuzziness is on G_{iF} for $i = 1, 2, 3, \dots, n$.
- ii. $G_F^2 = \{V, E_F\}$ where the edge set is fuzzy.
- iii. $G_F^3 = \{V, E(t_F, h_F)\}$ where both the vertex and edge sets are crisp, but the edges have fuzzy heads and tails.
- iv. $G_F^4 = \{V_F, E\}$ where the vertex set is fuzzy.
- v. $G_F^5 = \{V, E(w_F)\}$ where both the vertex and crisp sets are crisp but the edges have fuzzy weights.

The fact that crisp graph is a special case of a fuzzy graph can be stated in the following theorem.

Theorem 5.1 *Every crisp graph is a fuzzy graph.*

Proof Suppose $G(V, E)$ is a crisp graph. It can be considered as $G = (\sigma, \mu)$ which is a pair of function $\sigma : V \rightarrow \{0, 1\}$ and $\mu : V \times V \rightarrow \{0, 1\}$. It immediately fulfills the definition of fuzzy graph given by Rosenfeld [14] as well as definition given by Yeh and Bang [19]. \square

In view of Definitions 2.1 and 2.2 in Sect. 2, Theorem 5.1 leads to the following corollaries.

Corollary 5.1 *Every Autocatalytic Set is a fuzzy graph.*

Corollary 5.2 *Every Fuzzy Autocatalytic Set is also a fuzzy graph.*

The definition of fuzzy graph given in Definition 5.1 was designed to formulate a fuzzy graph for the clinical waste incineration process (see Fig. 2). The graph also happens to be FACS. In order to do that, we need to introduce several definitions.

Definition 5.2 Let $e_i \in E$. The fuzzy head of e_i denotes as $h(e_i)$ and the fuzzy tail $t(e_i)$ are functions of e_i such that $h : E \rightarrow [0, 1]$ and $t : E \rightarrow [0, 1]$ for $e_i \in E$. A fuzzy edge connectivity is a tuple $(t(e_i), h(e_e))$ and the set of all fuzzy edge connectivity is denoted as $C = \{(t(e_i), h(e_e)) : e_i \in E\}$.

In relation to our system, $t(e_i) = 1, \forall e_i$ since each variable was taken as a whole before it evolved to other variables. The membership value of fuzzy head (citealtSa05 is based on the reaction taken place and the strength of connection to the other variables in our system. By taking the membership value for each fuzzy edge connectivity as

$$\mu(e_i) = \min\{t(e_i), h(e_i)\} \quad (5.1)$$

in Theorem 4.1 (see Fig. 4), we can state the following theorem.

Theorem 5.2 *The graph for the clinical waste incineration process can be represented as $G_{d_f} = (V, E(\mu(e_i)))$ for $i = 1, 2, 3, \dots, 15$ where $\mu(e_i) = \min\{t(e_i), h(e_i)\}$.*

By Definitions 2.2 and 5.1, our fuzzy graph for the clinical incineration is an FACS as well as a fuzzy graph of Type 3 (see Fig. 5).

6 Implementation

The same color and thickness of each link in the crisp graph G_d (see Fig. 4) reveals that the connectivity between the vertices in the graph is the same. However, as compared to fuzzy graph G_{d_f} in Fig. 6, the greater the value of connectivity between the vertices, the thicker is the link between them. The different color signifies the different range of

Fig. 4 Crisp graph $G_d(V, E)$ of the incineration process

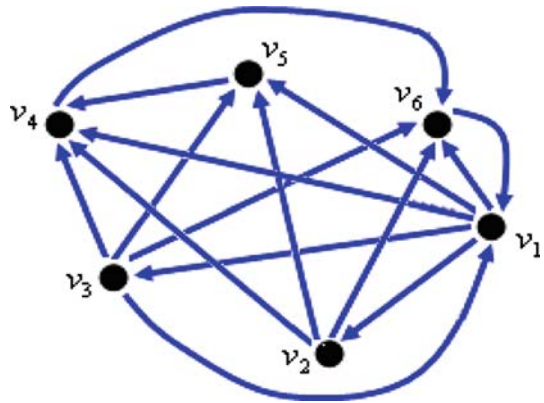


Fig. 5 Fuzzy head and tail

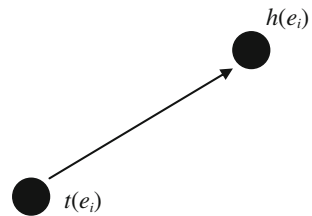
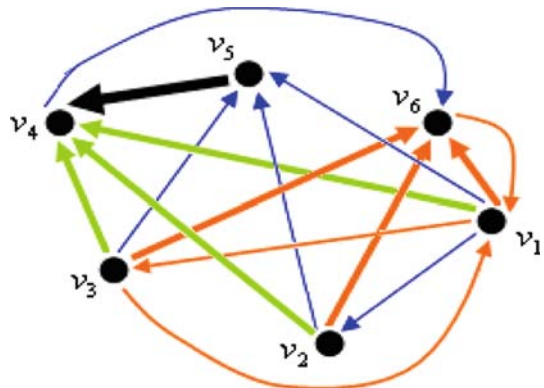


Fig. 6 Fuzzy graph of type 3 G_{d_F} for the clinical incineration process



membership value for the fuzzy edge connectivity. Thus, a difference in the result of the model would be expected since each model depends on the adjacency matrix of its graph. The graph dynamic procedure discussed, Sabariah [16] is applied to each graph. The results of concentration dynamics of the initial phase for both models are given in the following Table 1.

The rate of change of Fuel is negative for fuzzy graph as compared to the positive value for the crisp graph. The concentration value of Fuel should be decreasing as it was being consumed during the incineration process. Furthermore, the value obtained for CO by using fuzzy graph showed the formation of the gas is minimal in the incineration process. This is due to the assumption of perfect burning for the process.

Table 1 Comparison between models using crisp and fuzzy graph

x_i	Variable	Rate of change using crisp graph	Rate of change using fuzzy graph
1	Waste	−0.45300	−0.20671
2	Fuel	0.13600	−0.02952
3	O ₂	−2.49600	−0.57228
4	CO ₂	0.94500	0.56995
5	CO	0.94500	0.00002
6	H ₂ O & other pollutants	0.70900	0.23854

Table 2 Comparison between depletion sequence using crisp and fuzzy graph

	Crisp graph	Fuzzy graph
Sequence of depleted variables	Fuel, O ₂ , CO, CO ₂	Fuel, CO, O ₂ , waste
Products of process signified by the variables left at the end of procedure	Waste and H ₂ O & other pollutants	CO ₂ and H ₂ O & other pollutants

Moreover, the results of graph dynamics for both models can be compared by looking at the sequence of depleted variables and also the set of the variable left at the end of the procedure that signify the products of the incineration process as shown in Table 2.

The sequence of the variables removed from the system during the incineration process is more accurate for fuzzy graph as compared to the crisp graph. Fuzzy graph also indicated the products of the process as CO₂ and H₂O which confirmed to the real process as noted by Bruner [3].

7 Conclusion

Fuzzy Autocatalytic Set (FACS) has been defined and implemented in the modeling of the incineration process. The development of the theory has also been outlined in the paper along with the comparisons made to the results on both applications of crisp and fuzzy graph in the modeling. The results shown using this new concept prove to be more accurate than using crisp graph.

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