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# MATHEMATICAL MODELING OF A CLINICAL WASTE INCINERATION PROCESS

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## ABSTRACT

At present, there is no fundamentally based mathematical model of the incineration process of clinical waste. The development of an accurate mathematical model of the process is being hampered by the lack of measured data for validation due to its complexity feature. Due to the wide applications of the graph theory, a study was carried out to model a clinical waste incineration process using graph theory. Initially, a graphical model was constructed to explain the connections of the variables in the incinerator, which serves as a basis for a more dynamic graphical representation of the system. This model was found to be an Autocatalytic Set (ACS), conforming to the key feature of the model proposed by Jain and Krishna. Their model was then adopted and modified to suit the incineration process, which has resulted in a model explaining the two dynamics of the system. The former described the rate of change of the variables or species and the latter represented the evolution of the species in the incineration process.

## ABSTRAK

Pada masa kini, tiada suatu pun model matematik yang dapat dijadikan asas kepada model proses penunuan sisa buangan klinikal. Kelembapan dalam proses pembangunan model matematik ini disebabkan oleh ketiadaan data yang diperolehi daripada proses ini. Ketiadaan data ini pula berpunca dari ciri proses ini yang sungguh kompleks. Memandangkan keluasan penggunaan teori graf, suatu kajian telah dijalankan bagi memodelkan proses penunuan sisa buangan klinikal dengan menggunakan teori graf ini. Di peringkat awal kajian, satu model graf telah dibina bagi menerangkan hubungan pembolehubah dalam penunu dan graf ini menjadi asas kepada perwakilan graf yang lebih dinamik bagi sistem tersebut. Model ini didapati berbentuk Set Automangkinan (ACS) yang memuaskan ciri penting model yang dipelopori oleh Jain dan Krishna. Model mereka seterusnya telah digunapakai dan diubahsuai untuk dipadankan dengan proses penunuan. Ianya telah menghasilkan satu model yang menggambarkan kedua-dua dinamik proses penunuan, iaitu dinamik kepekatan dan dinamik graf bagi sistem tersebut. Dinamik kepekatan memerihalkan kadar perubahan pembolehubah atau spesis manakala dinamik graf menjelaskan evolusi spesis dalam proses tersebut.

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## **CHAPTER I**

# **INTRODUCTION**

## **1.1 Background and Motivation of Research**

In the past, clinical waste seemed not to receive much attention. However, with the emergence of deadly diseases such as AIDS and hepatitis B, it has been the area of increasing concern. In fact, the World Heath Organization (WHO) has initiated a number of activities to improve hospital waste management, particularly in developing countries (Ogawa, 1993). In Malaysia, such concern has resulted in clinical waste classified as a scheduled waste and controlled under Environmental Quality (Scheduled Waste) Regulations (Tan, 1989).

Clinical waste is defined as any 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, being waste which unless rendered safe may prove hazardous to any person coming into contact with it. It also includes such waste arising from medical, dental, veterinary, pharmaceutical or similar practice, investigation, treatment, care, teaching, or research, or collection of blood for transfusion, being waste that may cause infection to any person coming to contact with it.

Incineration is a process in which waste is burned under controlled condition to oxidize the carbon and hydrogen present in the waste. It has the advantage of converting waste into inert or less infectious material and at the same time reduces its volume up to 95% of its original size. Incineration is known to be the best available option for treating such wastes particularly the pathological related waste (Bruner, 1991). This is especially when there is limited land for landfill and gradual daily increase in the amount of waste generated by the public had made incineration more significant for waste disposal.

Although incineration is a preferred method of treatment, the air impurities associated with the burning of the waste is a major concern to the public. There is a rising sentiment, however, that waste incineration has serious drawbacks. While waste burn, chemical transformation is taking place. Organic compounds recombine, sometimes into chemicals that are toxic at extremely low concentrations (Reinhardt et. al, 1991). Polychlorinated dibenzo-p-dioxin (referred to as dioxin) and polychlorinated dibenzofurans (or furan) are two such toxic combustion products and, according to the United States Congressional Office of Technology Assessment (OTA, 1988)," concentrations of both dioxin and furans are considerably higher in hospital incinerator fly ash than in municipal incinerator fly ash."

Air monitoring or sampling apparatus at the stack of an incineration plant has been used routinely to check the emission levels and overall performance of an incinerator, but little insight is provided into the details occurring within the combustion chamber, that is, the incineration process (Lee, 1988; Kilgroe et al. 1990). Incineration process is one of the most complex unit operations presently in use. Obviously, the complexities associated with incinerator configuration, chemical and thermal interactions between the primary air and the waste, turbulence, and the heterogeneous characteristics of the waste itself have made the analyses and predictions in such a system quite difficult, and very few attempts appear in literature. Therefore mathematical modeling and numerical simulation for the incineration process are still not widely applied due to these complexities and they are still being developed (Goh et al. 1998; Klassen & Göerner. 1999). At present, there is no fundamentally based mathematical model of the incineration process of such waste. The development of an accurate mathematical model of the process is being hampered by the lack of measured data for validation due to its complexity feature. As such, the design, operation and control of incinerators are still based on crude empirical relations. Nevertheless, many attempts have been made to attain this fundamental mathematical model with such examples are the researches done by the group headed by Swithenbank of Sheffield University Waste Incineration Centre (SUWIC). Among others, the objective of the centre through its small scale incinerator plant is to identify the appropriate set of governing equations for combustion on the grate of an incinerator and to develop and validate a procedure for solving these equations (Yang et al. 2002). Consequently, the project will be use to all future research on incineration including the destiny of the contaminants since it will provide the upstream boundary conditions that are essential for understanding and modeling their subsequent fate.

The processes occurring within the combustion chamber of the incinerator include: pyrolysis, solid and gas combustion, conductive, convective and radiative heat transfer, mass transfer and gas flow through randomly packed beds of materials whose size, shape and orientation each is continuously changing (Swithenbank et al. 1997). In view of the complexity of the process, it is not surprising that the design of the incinerators has developed more as an art than a science. Hence, the many design variables for the incinerators had actually contributed to several modeling methods attempted in the modeling of the process. Furthermore, ensuring capital cost minimization, process efficiency and environmental friendliness of modern incineration plants had also initiated the growth of the modeling process in the field. Some examples of methods used in modeling the incineration process along with the models being developed so far could be seen in the following discussion.

Computational Fluid Dynamic (CFD) is the numerical analysis of fluid flow, heat transfer and related phenomena. CFD solvers contain a complex set of algorithms used for modeling and simulating the flow of fluids, gases, heat, and electric currents. Many technological advances in aeronautics, automobiles and space would not be possible without CFD. A number of modeling attempts concerning amongst others the combustion and radiation heat transfer, flow of temperature, flow of turbulence, gas flow and mixing behavior between waste and the combustion air of the incineration process using CFD have been reported (Nasserzadeh et al. 1993; Han et al. 1997; Swithenbank et al. 1997; Yang et al. 1999; Yang et al. 2003). Through CFD simulation of the combustion chamber of the incinerator, these problems are analyzed faster than by testing, in more detail, at an earlier stage in the design cycle for less money, and with lower risk.

Another method commonly used to advance the knowledge of flow structures, species distributions and mixing behaviors of turbulent burning in waste incineration process under various operating conditions is the Finite-Element Method (FEM) which was pioneered by R. Courant in 1943. Examples of such modeling attempts of the incineration process using FEM are Ravichandran & Gouldin (1992, 1993) who performed the numerical studies of two-dimensional (2D) isothermal flows in a typical configuration of a Municipal Solid Waste (MSW) Incinerator. Although their results show that mixing behaviors in combustion chambers are improved by properly arranged over-fire jets, no studies of the actual burning of waste were considered.

Chen and Tong (1997) also investigated the flame structures and species distributions within the combustion chamber of an MSW based on 2D simulation. The three-dimensional (3D) flow modeling of turbulent burning gases in an MSW using FEM were carried out by Chen at al. (1999). With the assumption of infinitely fast devolatilization of solid waste and non-uniformly distributed gaseous methane along the grate, burning flow structure are obtained by solving the governing differential equations of mean and turbulent quantities of velocity, temperature and species concentrations using a  $\kappa - \varepsilon$  turbulence model.

Other methods used in the modeling of the incineration process include the application of fuzzy logic and neural network theory. These theories are used especially in the optimization and control of the incineration process (Chen, 1995; Gierend & Born, 2000; Göerner, 2003; Fausett, 2000). Neural networks are also able to learn the behavior of a plant by looking at the process inputs and outputs.

Statistical method models are also used to understand, predict and forecast the incineration process. Such an example is the work of Nakamura et al. (2003) where Monte Carlo stochastic method has been applied to provide a time series description of the continuous variation of solid wastes at the feed end of the traveling grate. Sabariah et al. (2005) used linear regression model to determine the variables affecting the combustion efficiency of the incineration process. Fatmarini (2002) has used factor analysis to group the variables in the incineration process according to their specific communalities of same characteristic in order to understand the relationship between them.

The study concerning the chemical species within the incineration process has been reported by several researchers (Chen & Tong, 1997; Chen et al., 1999; Yang et al., 2003). The focuses of these studies are the species distribution and also the mixing of these species in the combustion chamber. Similar to the other modeling works mentioned above, the changes to these chemical species, namely, the changes in their concentrations during the incineration process has, not been reported. Thus, we are motivated to look at the changes in the concentration of the species or the variables such as the Waste, Fuel, Oxygen, Carbon Dioxide, Carbon Monoxide, Water and Other Pollutants during the process. The influencing elements that lead to the modeling method implemented in this study are discussed next.

## **1.2 Influencing Elements**

The chemical reaction taking place in the incineration process gives rise to complex webs of species or variables. These webs or networks signifying the evolution of these species could, in fact be represented by a mathematical model. A natural consideration to the study would be to indulge in graph theory and the following discussions elaborate the sequence of the considerations taken throughout the modeling work. Graph theory is a branch of mathematics that has real-world application in many areas, including industrial, electrical and transportation engineering, computer science, environmental conservation, management, marketing, scheduling, education, psychology, biology and chemistry (Chartrand, 1985; Evans and Minieka, 1992). Hence, due to its vast history of real world applications, the study resolved to graph theory in modeling the clinical waste incineration process. It is natural then that graphical models are constructed to represent the process and selection is made from these models to correlate with the dynamic nature of the process. Our emphasis in looking at the dynamics of the process is on the changes of the variables or the species in the system.

With this emphasis as our consideration, the evolution model that has graph theoretical concepts as its basis of model structure developed by Jain and Krishna (Jain and Krishna, 1998, 1999, 2001, 2002, 2003; Krishna, 2003) is adopted and modified in solving our problem. Autocatalytic Set (ACS) is the key feature of this model in looking at the dynamics of the system. The dynamics that are of concern here are the concentration dynamics of the species and the dynamics of the network change symbolized by the change of the graph. Two main theories incorporated in the construction of the model are the evolution theory and the theory of autocatalysis. How the species evolve and change in the system is determined by their autocatalytic interactions between them and this will be the main theme of the model.

#### **1.3** Statement of Problem

There is no fundamentally based mathematical model for the clinical waste incineration process (Swithenbank et al., 1997) and a wide range of different perspectives of the incineration process be investigated to make it an interesting platform to study. However, the main interest in this study would be on the changes of the species (variables) in the incineration system signifying the dynamics of the process. The emphasis is to model the dynamics of the clinical waste incineration process, so as, to understand the changes of the species that correlate to the actual process.

#### 1.4 Research Objectives

The main goal of the research is to model the clinical waste incineration process. To achieve these goals we have the following objectives as our working strategies. The objectives of the research are:

- To identify the parameters involved in the incinerator plant and construct a graphical model to represent the relationship between these parameters.
- To identify the variables (species) in the incineration process and to obtain a graphical model that would represent the dynamic of the system.
- To develop the mathematical model that has an autocatalytic set as the key feature and graph theoretical concept as the basis for the model.

#### **1.5** Scope of Research

For this research, our emphasis is on the incineration process of the incinerator plant. There are several different perspectives we could indulge in within the incineration process itself, but what interest us here is investigating the evolution of variables (species) in the process. The model of the incineration process will then aimed at investigating the changes to these variables involved in the process. The dynamic representation of the process shown by the model will be the main concern so as to represent its actual phenomenon.

Graph theoretic concepts and autocatalytic set would respectively constitute the basis and the key feature of the model. The model constructed would then be evaluated in term of its validity in explaining the real process.

#### **1.6** Summary and Outline of Thesis

The goal of the study is to model the clinical waste incineration process. The study is designated to achieve the goal with the objectives given in Section 1.4 which served as the guidelines of the research work resulting in the writing of this report. The outline of the report is given as follows.

Chapter 2 provides published literatures of different topics relevant to the study. It begins with examining the system and on identifying the problem. Here, brief history of incineration technology and an elaboration of Jain and Krishna's model (Jain and Krishna, 1998, 1999, 2001, 2002, 2003; Krishna, 2003) adopted in the study is given. This provides us with an insight on pursuing our problem-solving activity. Clinical waste incineration plant under study is reviewed to provide a background on the activities of the incineration process as well as on the parameters involved in the incineration plant. This chapter also introduces all the definitions, terminologies and concepts pertaining to the study which include the fundamentals of graph theory, flow and multicommodity flow model, autocatalytic set and dynamic model. These very basic concepts are introduced in the chapter to make sense of the problem-solving activities encountered in the study.

Chapter 3 presents the construction of the graphical models representing the incineration process. It begins with the discussion on the construction of a graph representing the connections between the parameters of the incinerator, which serves as the basic graph that generates the development of the subsequent graphs. An attempt to extend the work in the realm of flow theory to explain the incineration process is also discussed in the chapter. Subsequently, a detailed narration on the evolution of a graph that best explained the dynamic nature of the process is given.

Chapter 4 explains the framework of the model describing the clinical waste incineration process along with its implementation to the system. It explains the relation between the graphs, which is the basis for the model where the concept of autocatalytic set is the key feature of the model. The graph's relation to Perron

Frobenius Theorem is also described in this chapter. The results of the implementation of the model to the system are analyzed and discussed, in accordance to the actual process of the incineration system.

Chapter 5 summarizes the findings presented in the previous chapters and draws some conclusions from them. We end the chapter and the report with some recommendations for future research.

## **CHAPTER II**

## LITERATURE REVIEW

# 2.1 Introduction

This chapter reviews the related literature for the main theme of the research, that is modeling the incineration process using graph theoretical concept, begins in section 2.2 with the discussion on examining the system and identifying the problem. A brief description on the history of the incineration technology and the modeling progress of the incineration process provide an insight of the system as well as the problem. Depiction of the flow of the incinerator is also given. The discussion continues with the elaboration of the mathematical model proposed by Jain and Krishna. The discussion given in this section helps us to understand the relationship of the parameters in the process as well as to accommodate our justification to the consequent work in modeling the process.

The discussion then proceeds with the definition of mathematical modeling, its key features and how the modeling was carried out in general given in section 2.3. The discussion helps to understand the nature of mathematical modeling and its relation to the research work reported in this report.

# 2.2 Examining the System and Identifying the Problem

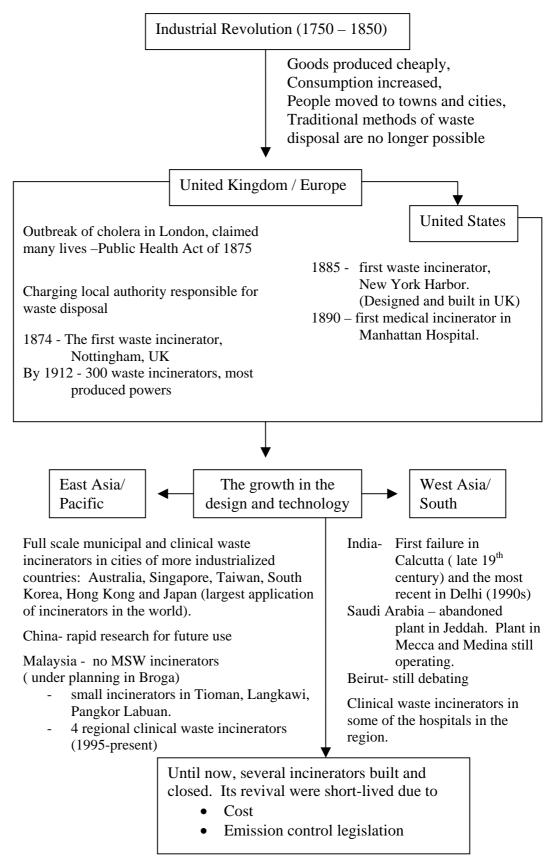
#### 2.2.1 Brief History of Incineration Technology

Throughout the early beginning history of mankind, various traditional methods were employed as waste disposal such as throwing it into pits around the farmhouse, open burning or it was used to feed the stocks. But not until the Industrial Revolution (1750-1850) where goods were produced cheaply, consumption increased and people moved to towns, that these traditional methods are no longer possible in the towns. As a result, the streets were full of piles of filth and garbage and this has led to the waste removal problem as well as the health hazard to the people. Municipal waste collection were then introduced where centralized dumping (landfill) site were encouraged. This also led to the introduction of the community waste incinerators in the late 1870s (Walsh, 2002).

The early period of incineration was marked by a series of problems and failures. The fundamental flaw of the plants was that they burned only the moist food waste fraction of the refuse and consequently operated at the low temperatures and required supplementary fuel, typically coal, to sustain combustion. Over the next half of the 20<sup>th</sup> century, a steady stream of design improvements stimulated the construction of incinerators throughout Europe and United States, resulting in peak waste combustion in many cities in mid-1930s. These early design advances, which raised combustion and operation efficiency to increase incinerator process rates and lower costs, culminated in 1950s with the introduction of completely mechanized municipal incinerators. Most of these incinerators programs collapsed when stricter emission standards were introduced in early 1970s.

Introduction of disposable diapers in 1966 and plastic packaging in 1970s had increased the amount of non-biodegradable waste and thus contributed to hazardous emission of toxic gaseous of dioxin and furan from the incinerators. Stringent measures given by the authorities to protect the environment, resulted in the growth of incineration studies and research centers aimed at developing better, efficient and safe incinerators. Since then, there existed evolution of incinerator design characteristics that had sustained its growth and also had hastened its decline throughout these years as illustrated by Figure 2.1. This is especially when there is limited land for landfill and gradual daily increase in the amount of waste generated by the public had made incineration more significant for waste disposal.

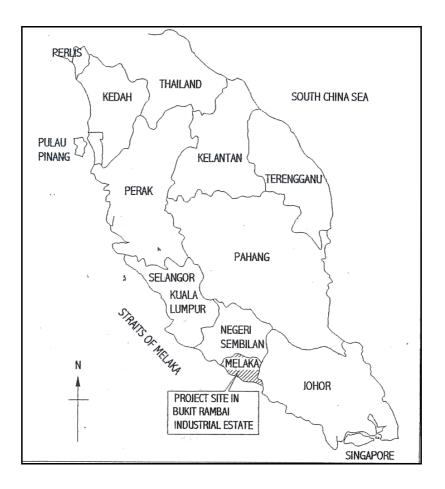
The scope of research in the incineration technology includes the incinerator design and building environment, optimizing the combustion processes and minimizing emission of toxic gases such as introducing the air pollution control facilities to incinerators. As a consequence, several models have been developed to understand and explain the incineration process. All these models have assisted in the control and the operation of the incinerators (as discussed in Section 1.1). We discuss in the next section the flow of the process in the clinical waste incineration plant we have selected for this study. The understanding of the flow of the process is vital for the development of the model of the clinical incineration process.



**Figure 2.1** Beginning and advancement of incineration technologies throughout various part of the world

#### 2.2.2 Clinical Waste Incineration Plant

In this research, information gathered from a clinical waste incineration facility in Bukit Rambai Industrial Estate, Malacca is used to model the incineration process. The structure of the plant together with the flow of the process based on the EIA report of the plant [EIA Report, 2000] is discussed. The plant is owned by Pantai Medivest Sdn. Bhd., which is formerly known as Tongkah Medivest Sdn. Bhd. It caters for the disposal of health related waste, mainly from the states of Malacca, Negri Sembilan and Johor (Figure 2.2). The plant is operating in full service ever since it was commissioned in 1997 (NST, August 21,2004).



**Figure 2.2** Location of the existing Pantai Medivest Sdn. Bhd. Incineration Plant in Malacca

Initially, the facility is equipped with two units of incinerators (each handling 250 kg waste/hr) served with common dry-wet air pollution control system which can handle one incinerator at any one time (the other incinerator serves as a standby unit). A bigger Air Control has been installed in March 2002 to handle both the incinerators. With this installation, both the incinerators can function at the same time and this has increased the throughput of waste to be incinerated, shorten the time and reduce the volume of waste to be stored in the refrigerated storage compartment. The existing facility is shown in Figure 2.3.



Figure 2.3The Incineration Plant owned by Pantai Medivest Sdn Bhd. inMalacca

# 2.2.2.1 Waste Burned

The facility is designated to incinerate clinical waste material of heterogeneous mixture of general refuse, laboratory and pharmaceutical chemicals,

containers, pathological waste and cytotoxic wastes. All of these wastes are potentially infectious. The clinical and physical characteristics of waste materials may vary widely. Similarly, clinical wastes can also vary considerably in composition, and consequently in heat release, moisture content and bulk density from one batch to the next.

Table 2.1 presents the typical waste characteristic that is being incinerated by the facility that can take a maximum of 250 kg of waste per hour only. The wastes are collected from various government or private hospitals or clinics throughout the states of Malacca, Negri Sembilan and Johor.

Material	%
P.V.C.	3
Pathological	5
Plastics other than P.V.C.	30
Paper including waxed paper	32
Hospital dressings, swabs, etc.	10
Miscellaneous (including flowers, rags, etc.)	10
Non-combustible including glass, metal etc.	10
Total	100

**Table 2.1**:Characteristics of waste burned

To date, the plants incinerates 130 ton of waste per month and the amount of incoming waste is increasing by 10% for the past few years ever since the plants started to operate. It is expected that the trend will continue as the number of hospital beds or population increase. Thus, the demand for a quick and efficient disposal of the waste will also need to keep up with this upward trend.

#### 2.2.2.2 The Incineration Plant Process Flow

The facility is designed with  $2 \times 250$ kg/hr incineration units. Each incinerator is equipped with both primary combustion chamber (PCC) with operating temperatures between 900<sup>o</sup>C and 1000<sup>o</sup>C, and secondary combustion chamber (SCC) with combustion temperature maintained over 1000<sup>o</sup>C using an auxiliary fuel burners. The PCC operates at high temperatures in order to achieve an efficient burnout of the waste while SCC further minimizes the remaining pollutants before passing through the flue gas cleaning system.

The flue gas cleaning or air pollution control system installed in the plant consists of a cooling tower (spray chamber) and a combination of dry-wet absorption system which includes a rotary contactor, cyclone, fabric filter, and wet scrubber unit. Appendix A presents the whole process flow of the incineration plant. We have reconstructed and simplified the diagram as in Figure 2.4 below.

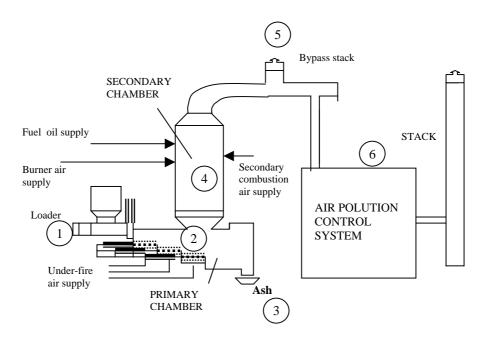


Figure 2.4 The Schematic Diagram of a Clinical Waste Incinerator

#### 2.2.2.3 Unit equipment of the Incineration Plant

The incineration plant consists of six sections. They are categorized as the following:

- 1. Loader and Bin Tippler,
- 2. Primary Combustion Chamber (PCC),
- 3. Ash Discharge System,
- 4. Secondary Combustion Chamber (SCC),
- 5. By-pass Stack,
- 6. Air Pollution Control System (APCS).

The location of each of these unit equipments is shown in Figure 2.8 corresponding to the number given in the figure.

#### i. Loader and Bin Tippler

The incinerator is equipped with hydraulic powered bin tippler which is capable of lifting the  $2 \times 240$  liter wheeled bin or any other designated type of container, tipping the contents directly into the incinerator loading hopper. The tippler is operable both automatically and manually controlled. The wastes are weighed before they are fed into the combustion chamber.

The loader is provided to allow the safe loading of waste materials into the incinerator whilst ensuring the following criteria:

- Minimal air leakage into the incinerator during load cycles.
- No fugitive emissions from loader during cycles.
- Minimal risks of fire in hopper.
- Minimization of molten plastic built-up in the loader area and subsequent jamming of fire doors.

As such, the loader is nicely arranged so that the slopping floor of the hopper will permit water to drain into the incinerator. The loader is automatically controlled to suit the process operating conditions. Undesirable operating conditions will automatically lock out the loader from operation to prevent further incineration of wastes.

#### ii. *Primary Combustion Chamber (PCC)*

The primary combustion chamber is a stepped hearth type consisting of three stationary hearths on which the waste burns. The stepped hearth design utilizes a series of rams to slowly push the waste material through the incinerator onto a burnout hearth for complete ash burnout. Each hearth is equipped with an ash pusher for the purposes of pushing the burning materials and clinker from the hearth. As the waste is pushed through the incinerator, it progressively burns to ash.

Each zone of the hearth is equipped with modulating combustion air supply and independent ash pusher controls. This allows total flexibility allowing the incinerator to operate efficiently as the properties of the waste may change in future. The final stage of the stepped hearth incinerator is the burnout hearth. It is on this hearth that carbonaceous matter generated in the controlled air environment gets in contact with excess air to burn out the carbon to an acceptable level.

Temperature control within the primary chamber is critical to prevent the melting and subsequent fusion of glass. The use of the stepped hearth type primary combustion chamber allows such temperature control. The primary chamber is constructed from a mild steel casing internally lined with refractory firebrick capable of withstanding in excess of the operating temperatures of  $800^{\circ}$ C -  $1000^{\circ}$ C. Auxiliary fuel burners are provided to ignite the wastes. Waste solids retention time in the primary chamber is adjusted in the range of 2 – 8 hours.

Whilst the incinerator primary chamber can operate under reducing or oxidizing modes, it is generally recommended that reducing conditions be maintained. Clinical waste being volatile and of high energy content is well suited to reduce air operation. Reducing conditions, commonly known as controlled air or starved air operation, involve using less than the required quantity combustion air necessary for complete destruction in the primary chamber. By starving the process air, the volatile components of the waste are gasified. The combustible gases produced can be considered to be a fuel and are mixed with air and completely combusted in the secondary chamber after ignition by a diesel burner in the ignition chamber.

The heavier components of the waste burned on the lower hearths and the burnout hearths provide heat for the pyrolysis process. The result is that energy from the waste is released throughout both chambers instead of mainly in the primary chamber as with multiple chamber and excess cooling air or water in the primary chamber and reduces the auxiliary diesel fuel requirement in the secondary chamber. Another advantage in the use of a two-stage combustion process is the significant reduction of nitrogen oxides emissions. The reduced quantity of primary air provides high retention times and low gas velocities in the primary chamber with the result that the entrainment and re-entrainment of particles is reduced considerably.

#### iii. Ash Discharge System

The incinerator combustion ashes are discharged from the primary chamber into water sealed trough for immediate quenching. These ashes are then removed from the trough by means of drag type ash conveyor.

#### iv. Secondary Combustion Chamber (SCC)

The exhaust gases from the primary combustion ignition chamber are drawn into the secondary combustion chamber. The SCC is lined with 230 mm thick low cement, high aluminum castable refractory which is capable of operating at the temperature of  $1300^{\circ}$ C. This zone is equipped with auxiliary diesel fuel burners. An auxiliary fuel burner is used to maintain the secondary combustion chamber temperature.

Combustion efficiency is assured by operating the secondary combustion chamber at 1000<sup>0</sup>C whilst maintaining an oxygen rich environment. The burners will re-ignite the partial products of combustion emitted from the primary chamber and

raise the temperature of the gases to in the excess of 1000<sup>o</sup>C. An efficient secondary chamber is essential to minimize emissions of dioxins and other products of incomplete combustion. The critical parameters when determining the efficiency of an incinerator secondary chamber are the combustion temperature, the chamber combustion time or residence time and the turbulence or contact time with excess air.

The secondary chamber is designed to provide a secondary chamber retention time of 2 seconds at a temperature of 1000<sup>o</sup>C and is capable of achieving combustion efficiencies in the order of 99.9999%. Combustion air is supplied by the secondary combustion air fan and is controlled to maintain an oxygen level of not less than 1%. The performance of the combustion process is monitored continuously using the flue gas analyzers, installed immediately after the chamber.

# v. Incinerator By-pass Stack

Each incinerator is provided with by-pass stack (immediately after the secondary chamber). This will allow bypassing of hot combustion gases directly from the incinerator to the atmosphere during incidents or in emergency situations. It is equipped with a fail-safe pneumatically assisted damper. During normal operation, this damper is fully closed allowing the combustion products to pass through the air pollution control system plant. In case of equipment failure, the stack cap opens up allowing the incinerator exhaust gases to discharge directly from the incinerator secondary chamber to the atmosphere.

This incinerator bypass stack is sufficiently height (that is 15 meters from the ground level) to ensure that the dispersion of emissions of pollutants during a bypass situation does not exceed acceptable levels. In the case of bypass, the feeding of wastes into the incineration is stopped immediately while waste already inside the chambers continue to burn. The incineration facility is equipped with a standby generator set to ensure that incineration process continues despite of power failure.

The importance of bypass: The incinerator is operating at negative pressure under all conditions, created by the induced draft (ID) fan. In the case of ID or APCS failure, the hot incinerator gases would be trapped within the incinerator chambers. Thus, creating a positive pressure build up in the chambers. Instead of drawing outside ambient air into the incinerator, as in the case of negative pressure, smoke fumes and even flames would escape from the incinerator at any and every possible opening. This will pose a serious risk of injury to the operator or building. In addition, a serious implication due to inhalation of partially combusted organic based gases particularly from the primary combustion chamber could be fatal in this case.

Thus, to overcome these difficulties every modern incinerator is equipped with this bypass facility, which shall only be activated during critical situation.

## vi. Air Pollution Control System (APCS)

There are eight fundamentals parts of the APCS installed in the plant. These are:

• Heat Exchanger

The function of the heat exchanger is to recover energy for the purpose of combustion air pre-heat and exhaust gas reheat.

• Adiabatic Gas Quench

The function of the adiabatic gas quench is to cool the incinerator exhaust gases to a temperature acceptable for entry into the fabric filter. This is achieved in down flow vessels into which the exhaust gases are contacted with finely atomized water droplets. The wastewater from the bin washing section is re-utilized and sprayed in this column.

Rotary Contactor Mixer

The function of the rotary contactor mixer is to ensure contact of the exhaust gases with lime and activated carbon. They are used for dioxin, acid gas and heavy metal control.

Cyclone Separator

The cyclone separator serves two functions; a particulate control device, and acts as a reactor chamber for lime and activated carbon to react with pollutants. It helps to increase the contacting time between the absorbent and the pollutant for better pollution control.

#### • Fabric Filter

The fabric filter is an efficient particulate control device and in this case, it also provides an additional contact surface for the exhaust gases particularly acid mist to react once the layer of absorbent is formed on the bag surface. This will complete the chemical neutralization process.

• Induced Draft Fan

The induced draft fan is used to provide the energy necessary to overcome the resistance to gas flow in the air pollution control plant. The inlet and outlet ductwork of this fan is equipped with noise attenuators. This fan is equipped with variables vanes for air flow control.

• Fluidized Bed or Packed Bed Scrubber

The function of the acid gas scrubber is to ensure that virtually all the acid gases generated in the incineration process are neutralized. The main scrubber casing, packing and internal pipe works are fabricated from a composite reinforced fiberglass. The scrubber is equipped with high efficiency packing and a preliminary mist elimination stage. The alkalinity of the fluidized bed scrubber liquor is continuously monitored using a pH sensor and is controlled by the addition of caustic soda. The wastewater from bin washing section is utilized as the scrubbing water and partly, channeled into the flue gas quench tower.

• Stack

Finally, the cleaned incinerator exhaust gas is pre-mixed and discharged through a 20 meter height stack, of 0.1m in diameter and at  $150^{\circ}$ C temperature.

The incineration plant can be further divided into two categories with the first five sections explained above known as the *incineration or combustion system* and the last section as the *air pollution control system*. The focus of this research is solely on the incineration process, thus two sections that are of concern in the study would be on the PCC and SCC of the incineration system. In the attempt of the research to understand the flow of the process and looking at the relationship of the input-output variables with the various components of the incineration plant, the APCS is also considered.

The study concerning the chemical species within incineration process has been reported by several researchers (Chen & Tong, 1997; Chen et al., 1999; Yang et al., 2003). The concentrations of these studies are the species distribution and also the mixing of these species in the combustion chamber. Actually, the chemical reactions taking place in the incineration process give rise to complex webs of species. The evolution of these species in fact can be represented using mathematical model. As such, a mathematical model of evolution proposed by Jain and Krishna (Jain and Krishna, 1998, 1999, 2001, 2002, 2003; Krishna, 2003) is discussed in the next section to perceive its relevance to our consequent work.

#### 2.2.3 Mathematical Model of Evolution Proposed by Jain and Krishna

Jain and Krishna proposed a simple mathematical model that captures some of the dynamics by which complex networks form. They treat the system as a directed graph whose nodes represent species and whose links represent the catalytic interactions among them. The populations of the species evolve according to the catalytic links between them and the graph (or network) itself, evolves by weeding out the least fit species. This model shows autocatalytic sets could lead to the inevitable growth of network complexity. Such sets first arise spontaneously by chance, and then attract other species to link up with them until all the species are linked to each other in an autocatalytic web with a much higher average connectivity and interdependence than before.

Eventually, the connectivity saturates in a statistical steady state. This provides some insight into how the chance appearance of certain structures (in this case autocatalytic sets) can suddenly accelerate the increase of network complexity. They found that an initially random graph also becomes highly structured as its complexity increases. The mathematical simplicity of the model allows them to determine analytically the timescales in the process as well as the level of non-randomness of the final network. Their work uses and extends some results in graph theory and the theory of non-negative matrices.

The model of Jain and Krishna are inspired by the work of Kauffman, Bagley and others who have explored questions about self-organization, the origin of life and some of the evolvability issues in work on artificial chemistries. In their research (Kauffman, 1983; Bagley et al. 1991), they have found that autocatalytic sets play an important role in the overall dynamics and suggested as one of the possible means by which a complex chemical organization, a 'metabolism', could have evolved on a prebiotic Earth.

The model analyzed by Jain and Krishna involves an evolving set of catalytically interacting molecules. The dynamical rules of the model attempts to capture key features of the evolution of chemical organizations on the prebiotic Earth. Such a set of molecules is an ideal example of a 'network' – a system of several interconnected components. The concept of a network is often used as a metaphor in describing a variety of chemical, biological and social systems (White et al., 1986; Faloutsos et al., 1999; Williams & Martinez, 2000; Fell & Wagner, 2000).

Graphs provide a natural way of representing networks in a mathematical model as evident from the studies listed above. This representation is useful for formulating questions about the structure and functioning of a network more precisely, as graph can suggest several quantities that can characterize its structure. As in many natural systems, the network of interactions is itself a dynamical variable. For instance, the transcription regulatory network of an organism changes as genes evolve, the World Wide Web changes as web pages get added and deleted, and ecosystems change as species become extinct and new species arise. With a graph representation of the network, one can model processes that alter the graph with time, either in discrete steps or continuously.

Representing this network as a graph makes it possible to use various graphtheoretic measures to characterize its structure. These measures may include the degree distribution and the eigenvalue spectrum of a graph. A structural characteristic that is of interest in the model, especially for chemical networks, is of *autocatalysis*. The concept of autocatalysis comes from chemistry. A catalyst is a substance that facilitates a chemical reaction without being permanently changed. In autocatalysis, a product of a reaction serves as a catalyst for that same reaction. An *autocatalytic set* is a set of reactions that are not individually autocatalytic, but whose product catalyzes one another. The result is that the behaviors of the reactions in the set are correlated with one another. If reaction A speeds up (say due to an increased supply of its reagents), so does any reaction catalyzed by the products of A. If A slows down, so do its autocatalytic partners.

Hong et al. (1992) and Lee et al. (1997) have constructed a pair of different molecules that catalyze one another's (as well as their own) production and hence form an autocatalytic set. Wächterhäuser (1990) and Morowitz et al. (2000) use a slightly different, but related, definition of autocatalysis to argue that the reductive citric acid cycle is autocatalytic. Jain and Krishna (1998) have given a graphtheoretic definition of autocatalytic set and is discussed in section 3.5. The connection between autocatalytic set and field of mathematics, is realized by the establishment of random graphs by Erdos and Rényi (1960). Autocatalytic set play a major role in the dynamics of the model studied by Jain and Krishna. Figure 2.5 illustrates the chronological development of autocatalytic set from its encapsulation up to the point where Jain and Krishna had adopted the theory in their study.

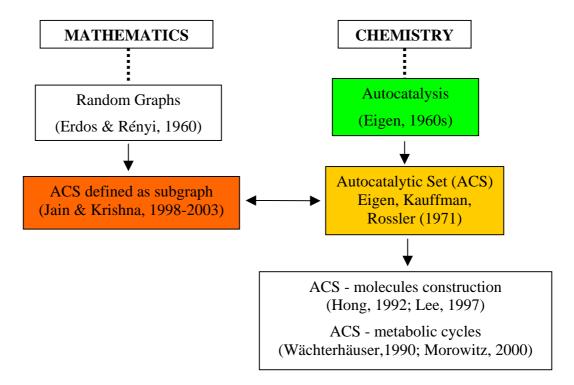


Figure 2.5 History and development of the theory of ACS

Another feature of the network that is of concern to Jain and Krishna in the study is the dynamics of variables 'living' on the graph in which is affected by the network topology. Examples of such networks are the food-web structure of an ecosystem which affects the dynamics of its constituent species' populations and the network of human contacts which influences the spread of a contagious disease. These dynamical systems on networks are often modeled as a set of coupled differential equations in which the couplings are specified by the network of interactions (Kaneko, 1989; Pérez et al., 1996; Strogatz, 2000; Sinha, 2002; Bhalla, 2002). In some systems it is more appropriate to represent the dynamics by difference equations, rather than differential equations, or by cellular automata. This is especially true for systems where the variables of interest take discrete values and assuming them to be continuous variables is a bad approximation (Arbib, 1995; Nagel, 2003). Here, Jain and Krishna has modeled the dynamics as a set of coupled differential equation and this will be discussed in Section 3.5.2.

When the dynamics can be assumed to be reaching some steady state or fixed point, there may be short cuts to finding the steady state without actually having to solve the equations of motion. Jain and Krishna have taken the attractor to the dynamic of their network to be the Perron Frobenius Eigenvector of the system and is shown in Section 3.5.3. The focus of the model was not only on the dynamical systems on fixed network but also on the dynamic network. This is in consideration that real networks are rarely static. While studies of static networks do provide some insight into network evolution, it is natural to address such evolution-related questions in models where the network is also a dynamical variable. An obvious question, therefore, is how (and why) did a particular network evolve into the specific structure we see? For instance, has the structure of a network evolved to optimize certain functionality or rather what are the mechanisms that cause the network to change? Such changes or the dynamics of the networks are reported in several studies (Watts & Strogatz, 1998; Fell & Wagner, 2000, Albert et al. 2000; Krishna, 2003).

In summary, Jain & Krishna has addressed some of these issues within the context of a specific mathematical model of an evolving network. Many of the

phenomena exhibited by the model are reminiscent of the phenomena seen in variety of evolving networks. Such phenomena are the growth of non-random structure (in the form of autocatalytic sets), the growth of independence and cooperation between nodes of the network, sudden mass extinctions due to the extinction of keystone species or the creation of certain new structures in the network. The model provides a simple mathematical framework within which to analyze the mechanisms that produce such phenomena. The basic model, and its variants, will be specific instances of a broad framework for modeling evolving networks given in the following table (Table 2.2).

<b>Table 2.2</b> :	Framework of a model in which the network co-evolves with other
variables (add	ppted by Jain and Krishna)

The dynamical variables are a directed graph <i>C</i> and a variable $x_i$		
associated with each node <i>i</i> of the graph.		
To start with, the graph <i>C</i> and the variables $x_i$ are given some initial		
values. The particular choice of values will depend on the system being modeled.		
Step 1: First, keeping the graph ( $C_{n-1}$ at step <i>n</i> -1) fixed, the $x_i$		
evolved for a specified time <i>t</i> according to a set of differential equations that can be schematically written in the form: $\dot{x}_i = f_i(C_{n-1}, x_1, x_2,)$ where $f_i$ are certain functions		
that depend upon the graph $C_{n-1}$ and on all the $x_i$ variables.		
Step 2: After this, some nodes may be removed from the graph, along with their links. Some links may also be removed from the graph. Which nodes and links are removed will, in general, depend on the $x_i$ values of the nodes and the graph $C_{n-1}$ .		
Step 3: Similarly, some nodes may be added to the graph. These new nodes will be assigned links with existing nodes. The rules for specifying which links will be assigned may depend on the $x_i$ variable, which will be assigned some initial value. Some new links may be added between existing nodes, which again may depend on the $x_i$ values of the nodes and $C_{n-1}$ .		

The framework above considers a process that alters a network, represented by a graph, in discrete steps. The series of graphs produced can be denoted as  $C_n, n = 1, 2, ...$  Each step of the process, taking a graph from  $C_{n-1}$  to  $C_n$ , will be called a 'graph update event'. The framework therefore defines a class of evolving network models that consist of a graph evolving, by a series of graph update events, along with other system variables. Two time-scales can be represented by the framework, in which the dynamics connotes the short time scale whereas the graph updates indicates the changes in the network and thus represent the longer time-scale.

The difference in the model we are developing in this study as compared to the one done by Jain and Krishna (as shown in Table 2.2) is that the nodes removed from the network are irreplaceable. This is in the consideration that certain variable depleting at each stage of the incineration process. The model is based on graph theoretical concept and basic concepts of the theory will be discussed in the Chapter 3. Next, we present the Definitions and Terminologies that would help us to understand the whole process of the research.

### 2.3 Definitions and Terminologies

### 2.3.1 Graph Theory

Any situation that can be described by a set of elements and a relationship between pairs of elements can be described by a graph. A graph consists of a set of points and a set of lines connecting those points (Epp, 1993). The points are referred to as vertices or nodes and the lines as edges or links. Edges can have directionality and those graphs associated with them are called directed graphs. Throughout this thesis, we will be concentrating on this type of graph. Henceforth, we will use the term 'graph' to refer to a labeled, directed graph. For the convenience of the reader, we introduce some basic elements of graph theory (Harary, 1969; Foulds, 1991; Jain and Krishna, 2003). We set out the notation that will be used and give definitions of directed graphs, adjacency matrices, subgraphs, degree of a node, paths and cycles. Eulerian circuit, Eulerian trail, Hamiltonian of a graph are also narrated here.

# 2.3.1.1 Directed Graphs, Adjacency Matrices and Degrees

### **Definition 2.1**: Directed graph

A directed graph G = G(V, E) is defined by a set of V of "vertices", also known as "nodes", and a set E of "edges" or "links", where each edge is an ordered pair of vertices.

The set of nodes can be conveniently labeled by  $V = \{v_1, v_2, \dots, v_s\}$  for a directed graph of *s* nodes. A graph with *s* nodes is completely specified by an  $s \times s$  matrix,  $C = (c_{ij})$ , called the "adjacency matrix" of the graph, and vice versa.

# **Definition 2.2**: Adjacency Matrix

The adjacency matrix of a graph G = G(V, E) with *s* nodes is an  $s \times s$  matrix, denoted by  $C = (c_{ij})$ , where  $c_{ij} = 1$  if *E* contains a directed link (j,i) (arrow pointing from node *j* to node *i*), and  $c_{ij} = 0$  otherwise.

This convention given by Jain and Krishna differs from the usual one (Harary, 1969; Robinson and Foulds, 1980: Bollobás, 1998) where  $c_{ij} = 1$  if and only if there is a link from node *i* to node *j*; the transpose of the adjacency matrix defined above. They chose this convention because it is more convenient in the context of the dynamical system and due to its relevancy to our dynamical system, we have also adopted this definition and will be discussed in Chapter 5. We will use the term "graph" and "adjacency matrix" interchangeably. The phrase "a graph with adjacency matrix *C*" will often be abbreviated to "a graph *C*".

**Definition 2.3**: Subgraph

A graph G' = G'(V', E') is called a subgraph of G = G(V, E) if  $V' \subset V$  and  $E' \subset E$ .

**Definition 2.4**: Degree, in-degree and out-degree

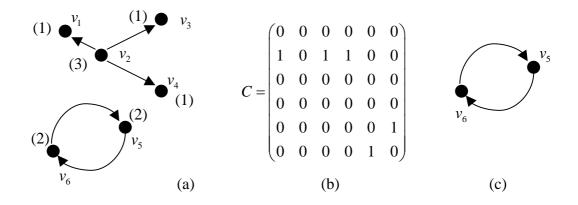
The degree, or total degree, of a node is the total number of incoming plus outgoing links from that node, that is, the total degree of node i is

$$\sum_{j=1}^{s} \left( c_{ij} + c_{ji} \right).$$

The in-degree of a node is the total number of incoming links to that node, that is, the in-degree of node *i* is  $\sum_{i=1}^{s} c_{ii}$ .

The out-degree of a node is the total number of outgoing links from that node, that is, the out-degree of node *i* is  $\sum_{i=1}^{s} c_{ji}$ .

Figure 2.6 shows the example of a graph, its adjacency matrix and subgraph.



**Figure 2.6** (a) A graph C (b) An adjacency matrix of graph C (c) A subgraph of graph C

For the graph C in Figure 3.1(a), the bracketed number adjacent to each node indicates the degree for each node. We could see that the total degree of C is 10 that is twice the number of nodes in C (Epp, 1993).

# 2.3.1.2 Walks, Paths and Cycles

**Definition 2.5**: Walk, closed walk

A walk of length *n* (from node  $v_1$  to node  $v_{n+1}$ ) is an alternating sequence of vertices and edges  $v_1e_1v_2e_2 \dots v_ne_nv_{n+1}$  such that edge  $e_1 = (v_1, v_2), e_2 = (v_2, v_3)$  and so on. If  $v_1 = v_{n+1}$ , it is known as a *closed walk* or *circuit*.

The existence of even one closed walk in the graph implies the existence of an infinite number of distinct walks in the graph. In the graph of Figure 3.1(a), there infinite number walks (for are of from  $v_5$  to  $v_6$ example,  $v_5 \rightarrow v_6, v_5 \rightarrow v_6 \rightarrow v_5 \rightarrow v_6, \dots$ ) but no walk from node  $v_5$  to  $v_2$ . If C is the adjacency matrix of a graph then it is easy to see that  $(C^n)_{ii}$  equals the number of distinct walks of length *n* from  $v_j$  to  $v_i$ . For example,  $(C^2)_{ij} = \sum_{k=1}^{s} c_{ik} c_{kj}$ ; each term in the sum is unity if and only if there exists a link from  $v_i$  to  $v_k$  and from  $v_k$  to  $v_i$ , thus the sum counts the number of walks of length 2 from  $v_j$  to  $v_i$ .

# **Definition 2.6**: Path

A walk with all nodes distinct is a path

### **Definition 2.7**: Cycle, *n*-cycle

An *n*-cycle is a closed walk with *n* links, and all intermediate nodes distinct.

The term 'cycle' is also referred to the subgraph consisting of the nodes and links that form the cycle. Thus any subgraph with  $n \ge 1$  nodes that contain exactly n links and also contains a closed walk that covers all n is an n-cycle. For an example, the subgraph induced by nodes  $v_5$  and  $v_6$  in Figure 3.1(a) is a 2-cycle. Clearly any graph that has a closed walk contains a cycle.

# 2.3.1.3 Connectedness, Euler Circuit, Euler Trail and Hamiltonian of a Graph

### **Definition 2.8**: Connected graph

A graph C, is termed connected if for every pair of vertices in C are joined by a path and is termed disconnected if it is not connected.

# **Definition 2.9**: Euler circuit

A graph *C* has an *Euler circuit* if and only if *C* is connected and every vertex of *C* has even degree.

# **Definition 2.10:** Eulerian trail

A graph *C* has an *Eulerian trail* if and only if *C* contains vertices  $v_i$  and  $v_j$  such that

out-degree  $v_i$  = in-degree  $v_j$  + 1 and in-degree  $v_j$  = out-degree  $v_i$  + 1 and out-degree  $v_k$  = in-degree  $v_k$  for all other vertices  $v_k \in C$ .

Furthermore the trails begins at  $v_i$  and ends at  $v_j$ .

# **Definition 2.11**: Hamiltonian circuit

A Hamiltonian circuit for a graph C is a simple circuit that includes every vertex of C.

## **Proposition 2.1:**

If a graph C has a Hamiltonian circuit, then C has a subgraph H with the following properties:

- (i) H contains every vertex of C,
- (ii) H is connected,
- (iii) *H* has the same number of edges as the number of vertices,
- (iv) Every vertex of *H* has degree 2.

The adjacency matrix of the graph discussed in this thesis will be of a nonnegative matrix. Many properties and characteristics of this type of matrix will be looked into in our problem, thus our next discussion is on the non-negative matrix.

### 2.3.2 Non-negative Matrices

Square matrices whose entries are all nonnegative (all entries in them are 0 or greater) have special properties. Such matrices are mostly common in describing the world real phenomenon or models. Works and results on such type of matrices have wide dispersal of applications into the many fields of science. This includes the Perron's 1907 result, which was later extended by Frobenius work and eventually known collectively as Perron-Fobenius Theorem (MacCluer, 2000). The results of the Perron-Frobenius (PF) Theorem depend upon what kind of the nonnegative matrix. The matrix of interest here is called *irreducible* (Seneta, 1973; Varga, 1962).

# **2.3.2.1 Irreducible Graphs and Matrices**

# **Definition 2.12**: Irreducible graph

A graph is termed irreducible if each node in the graph has access to every other node.

The simplest irreducible subgraph is a 1-cycle. In Figure 3.1(a), the subgraph induced by  $v_5$  and  $v_6$  is irreducible, but the subgraph induced by  $v_1$ ,  $v_2$ ,  $v_3$  and  $v_4$  is not irreducible as there is, for example, no path from  $v_4$  to  $v_3$ .

**Definition 2.13**: Irreducible matrix

A matrix *C* is irreducible if for every ordered pair of nodes  $v_j$  and  $v_i$ , there exists a positive integer k such that  $(C^k)_{ii} > 0$ .

Thus, if a graph is irreducible then its adjacency matrix is also irreducible, and vice versa. Irreducible graphs are, by definition, strongly connected graphs. In fact, all strongly connected graphs are irreducible, except the graph consisting of a single node with no link (by definition it is called a trivial strongly connected graph) which is not irreducible.

### 2.3.2.2 Perron-Frobenius Eigenvectors (PFE)

### 2.3.2.2.1 The Perron-Frobenius Theorem

The Perron-Frobenius Theorem for irreducible matrices states (Seneta, 1973; MacCluer, 2000):

Suppose T is an  $s \times s$  non-negative irreducible matrix. Then there exists an eigenvalue r such that:

- (i) r is real and positive;
- (ii) with r can be associated strictly positive eigenvectors;
- (iii)  $|r| \ge |\lambda|$  for any eigenvalue  $\lambda$ ;
- (iv) the eigenvectors associated with *r* are unique to constant multiples;
- (v) r is a simple root of the characteristic equation of T.

# **Definition 2.14**: Perron-Frobenius eigenvalue

For any irreducible graph *C*, the eigenvalue of *C* that is real and larger than or equal to all other eigenvalues in magnitude will be called the Perron-Fobenius eigenvalue of the graph and denoted by  $\lambda_1(C)$ .

**Definition 2.15**: Perron-Frobenius Eigenvector (PFE)

For any graph *C*, the eigenvector corresponding to  $\lambda_1(C)$  consisting only of real and non-negative components will be referred to as Perron-Frobenius eigenvector (PFE).

It is noted that the Perron-Frobenius Theorem guarantees the existence of such an eigenvalue and also the existence of at least one such eigenvector.

The Perron-Frobenius eigenvalue of the graph in Figure 3.1(a) is 1 and  $(0 \ 0 \ 0 \ 0.7071 \ 0.7071)^T$  is the Perron-Frobenius eigenvector. The presence and absence of closed walks in a graph can be determined from the Perron-Frobenius eigenvalue of its adjacency matrix as given by the following proposition (Jain and Krishna, 1998; 1999; 2000; 2003; Krishna, 2003).

### **Proposition 2.2**:

If a graph C

- (i) has no closed walk then  $\lambda_1(C) = 0$ ,
- (ii) has a closed walk then  $\lambda_1(C) \ge 1$ .

Here,  $\lambda_1$  cannot take the value between zero and one due to the discreteness of the entries of *C*, which are either 0 or 1. But when the values of the entries are in the interval [0,1], then  $\lambda_1$  will take the value between 0 and 1 and will be discussed in Chapter 6. A natural consequence of exploring into the network system where graph theory forms the basis of it is to indulge in flow modeling. A brief review on the topic will be discussed since our work will not resort to flow model in depth due to the reasons explained in the Chapter 4.

# 2.3.3 Flow Model and Multicommodity Flow Model

Network flow is a problem domain that lies at the cusp between several fields of inquiry, including applied mathematics, computer science, engineering, management, and operational research. The field has a rich and long tradition, tracing its roots back to the work of Gustav Kirchhof and other early pioneers of electrical engineering and mechanics who first systematically analyzed electrical circuits. This early work set the foundations of many of the key ideas of network flow theory and established networks (graphs) as useful mathematical objects for representing many physical systems (Gomory & Hu, 1975; Ahuja et al., 1993).

Often, the aim of a study is to maximize the amount of a quantity transported from one place to another. At other times is to determine the least-cost way to send a given quantity from the source to the destinations (sinks). Conservation of flow is fundamental to network flow problems. Flow in from the source equals flow out from the sink. Similarly, conservation applies to flows into and out of all vertices of the networking. For the maximum-flow problem, the total flow between a source vertex and a sink vertex is maximized, subject to capacity constraints that limit the allowable flow through each edge.

# **Definition 2.16**: Source, sink and arc flow

The *source* is the entry of flow to the network and the *sink* is the exit of flow from the network.

The *arc flow*  $x_{ij}$ , and in particular the flow  $x_{sj}$  from the source and  $x_{it}$  into the sink, are defined as a set of non-negative numbers satisfying the following constraints:

$$\sum_{i} x_{ij} - \sum_{k} x_{jk} = \begin{cases} -v & \text{if } j = s \\ 0 & \text{if } j \neq s, t \\ v & \text{if } j = t \end{cases}$$

Multicommodity flow problems on the other hand arise when several commodities use the same underlying network (Ahuja et al., 1993). The commodities may either be differentiated by their physical characteristics or simply by their origin to destination pairs. Different commodities have different origins and destinations and commodities have separate mass balance constraints at each node. However, the sharing of the common arc capacities binds the different commodities together. The essential issue addressed by the multicommodity flow problems is the allocation of the capacity of each arc to the individual commodity in a way that minimizes the overall flow cost.

Examples of multicommodity problems are:

- the transportation of passengers from different origins to different destinations within a city,
- the routing of nonhomogeneous tankers (non-homogeneous in terms of speed, carrying capacity and operating cost),
- the worldwide shipment of different varieties of grains (such as corn, rice and soybean) from countries that produce the grains to the countries that consume them,
- the transmission of messages in a communication network between different origin-destination pairs.

#### 2.3.4 Construction of the Clinical Waste Incineration Process Model

The model will be constructed based on Jain and Krishna's model (Jain and Krishna, 1998; 1999; 2001; 2002; 2003; Krishna, 2003). The key feature of the model is the autocatalytic set and will be discussed in Section 2.3.4.1. The other important feature is the dynamics of the variables in the network. In this thesis, we have opted for a set of coupled differential equation as the dynamic model for the population dynamics as explained in Section 2.3.4.2. This led to the discussion on attractor of the dynamics in Section 2.3.4.3.

### 2.3.4.1 Autocatalytic set

The concept of autocatalytic set (ACS) was first introduced in the context of a set of catalytically interacting molecules, where it was defined to be a set of molecular species that contains, within itself, a catalyst for each of the member species (Eigen, 1971; Kauffman, 1971; Rossler, 1971). As we have explained in section 2.4.3, Jain and Krishna has initiated the autocatalytic set in terms of graph-theoretical concept. Imagining a node in a directed graph to represent a molecular species and a link from j to i as signifying that j is a catalyst for i, has motivated the following graph-theoretic definition of an Autocatalytic Set [Jain and Krishna, 1998] in any directed graph.

# **Definition 2.17**: Autocatalytic set (ACS)

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

We have illustrated the development of research on autocatalytic set up to its initiation to graph theoretic concept by Jain and Krishna (Figure 2.8) in the previous chapter. Figure 3.1 below illustrates the application and extension made to the concept of ACS in this research to model the clinical incineration process.

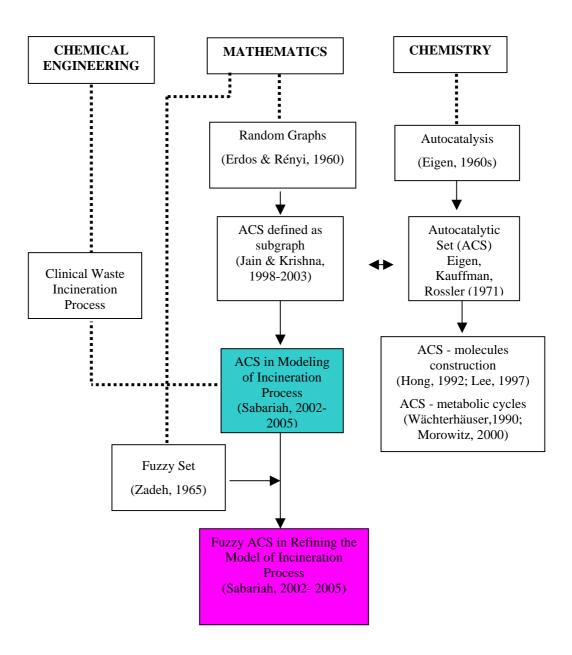
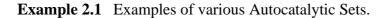


Figure 2.7 Extension of the theory of ACS in this study

Few examples of ACSs are illustrated in Figure 2.8. The simplest form of an ACS is a 1-cycle, Figure 2.8 (a). Figures 2.8a and 2.8b are graphs that irreducible as well as cycles, 2.8c is an ACS that is not irreducible subgraph and hence not a cycle, while 2.8d and 2.8e are examples of irreducible graphs that are not cycles.



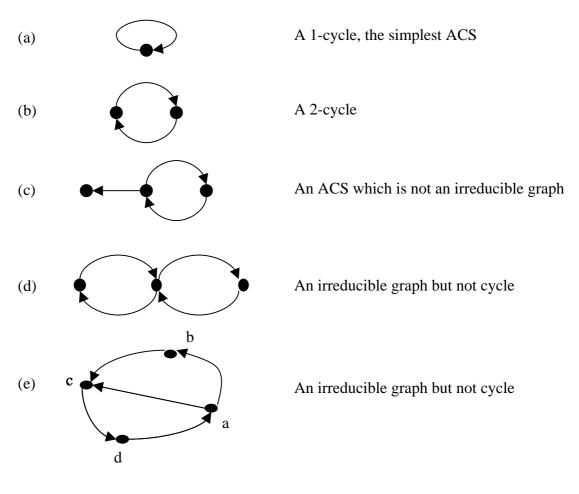


Figure 2.8 Examples of Autocatalytic Sets

There is hierarchical relationship between cycles, irreducible subgraphs and ACSs. This is shown in the following propositions (Jain and Krishna, 1998; 1999).

# **Proposition 2.3:**

- (i) All cycles are irreducible subgraphs and all irreducible subgraphs are ACSs.
- (ii) Not all ACSs are irreducible subgraphs and not all irreducible subgraphs are cycles.

The ACS is a useful graph-theoretic construct in its connection with the PFE. Firstly, the Perron-Frobenius eigenvalue of a graph is an indicator of the existence of an ACS in the graph.

#### **Proposition 2.4:**

An ACS must contain a closed walk. Consequently, the following is true.

- (i) If a graph C has no ACS then  $\lambda_1 = 0$ .
- (ii) If a graph C has an ACS then  $\lambda_1 \ge 1$ .

Let **x** be a PFE of a graph. Consider the set of all nodes *i* for which  $x_i$  is nonzero. Here, Jain and Krishna (1998, 1999) has denoted the subgraph induced by these nodes as the 'subgraph of the PFE **x**'. If all the components of the PFE are non-zero then the subgraph of the PFE is the entire graph. Consequently, Jain and Krishna put forward the following proposition.

# **Proposition 2.5:**

If  $\lambda_1 \ge 1$ , then the subgraph of any PFE of *C* is an ACS.

# 2.3.4.2 Dynamic Models

Dynamical systems on networks are often modeled as set of coupled differential equations, in which the couplings are specified by the network of interactions (Strogatz, 2000; Kaneko, 1989; Gade et.al. 1995; Jain and Krishna, 2003b). Other examples of representation of dynamical systems are Lotka-Voltera equation, replicator equation and also some complicated differential equations (Drossel and McKane, 2003). Certain systems are more appropriately represented as difference equations. In particular, this is true for systems where the variables of interest take discrete values. For such system, assuming them to be continuous variables is a bad approximation (Nagel, 2003; Arbib, 1995).

The dynamical system of interest in the study is the following set of coupled differential equation:

$$\dot{x}_{i} = \sum_{j=1}^{s} c_{ij} x_{j} - x_{i} \sum_{j,k=1}^{s} c_{kj} x_{j}$$
(2.1)

where  $C = (c_{ij})$  is a fixed graph with *s* nodes.

Note that the dynamics preserves the normalization of  $\mathbf{x}$ , that is:

$$\sum_{i=1}^{s} \dot{x}_i = 0.$$
 (2.2)

Equation 2.1 has been used by Eigen et. al. (1989) to describe the dynamics of the relative populations of self-replicating string and also by Jain and Krishna (2003) in their analysis of a model of an evolving set of catalytically interacting molecules. The system as denoted by the equation gives rise to a set of linear change in the  $x_i$  variables.

The model contains another dynamical variable  $\mathbf{x} \equiv (x_1, x_2, ..., x_s)$  where  $x_i$  stands for the relative population of the *i*<sup>th</sup> variable. The set of variables  $x_i$  can be thought of as 'living' on the nodes of the graph. The time evolution of  $\mathbf{x}$  depends upon the interaction coefficients *C*, as is usual in the population models. Each variable has a concentration  $y_i$  in the system. Relative concentration for each of the variables is given by

$$x_i \equiv y_i / \sum_j y_j . \tag{2.3}$$

By definition, we have

$$\sum_{i=1}^{s} x_i = 1, \quad \text{for } 0 \le x_i \le 1.$$
(2.4)

Equation 3.1 follows from the rate equation

$$\dot{y}_i = \sum_j c_{ij} y_j - \phi y_i$$
(2.5)

where  $\phi(t)$  is some function of time *t*. It is a simple idealization of rate equations in a well-stirred chemical reactor (Ashmore, 1963).

The first term of Equation 2.1 follows by taking the derivative of Equation 2.2 (Jain and Krishna, 1998; 1999; 2001; 2002; 2003; Krishna, 2003). The second (quadratic) term in Equation 2.1 follows directly from Equation 2.4 and the nonlinear relationship between  $x_i$  and  $y_i$ . Physically it is needed to preserve the normalization of the  $x_i$  under time evolution. When negative links are permitted, the second term of Equation 2.1 is needed in general to prevent relative concentration from becoming negative.

The changing of variables experienced in this dynamics stage is expected to reach its stable state at a certain time t. This equilibrium state to which all the variables converge is known as an **attractor**. An attractor attracts different possible state of the system, so that all trajectories come together at the same point. The key to changing of network that will be discussed in Chapter 5 and 6 is on the **selection** of the variables to be removed from the existing network. The selection made would depend on the choice of the attractor to the model. The following subsection introduces the proposition made by Jain and Krishna to explain their choice of an attractor for the population dynamics of their model (Jain and Krishna, 2001).

### 2.3.4.3 Attractors of the Population Dynamics

An attractor for a fixed graph  $C = (c_{ij})$  with *s* nodes, considered by Equation 3.1 with the simplex of normalized non-negative vectors in *s* dimensions:

$$J = \left\{ \mathbf{x} \equiv (x_1, x_2, \dots, x_s) \in \Re^s \, \middle| \, 0 \le x_i \le 1, \, \sum_{i=1}^s x_i = 1 \right\}$$

is presented by the PFEs (Jain and Krishna, 2001). In this study, the proposition put forward by Jain and Krishna in particular their choice of an attractor for their work is adopted.

**Proposition 2.6** Attractor of Equation 2.1 (Jain and Krishna, 2001)

For any graph *C*,

- i. Every eigenvector of C that belongs to J is a fixed point of Equation 2.1 and vice versa.
- ii. Starting from any initial condition in the simplex J, the trajectory converges to some fixed point (generically denoted X) in J.
- iii. For generic initial condition in J, X is Perron-Frobenius eigenvector (PFE) of C. (For special initial conditions, forming a space of measure zero in J, X could be some other eigenvector of C. Henceforth we ignore such special initial conditions.)
- iv. If C has a unique PFE, X is the unique stable attractor of Equation 2.1.
- v. If *C* has more that one linearly independent PFE, the *X* can depend upon the initial conditions. The set of allowed *X* is a convex linear combination of a subset of the PFEs.

The interior of this convex set in J may then be said to be the "attractor" of Equation 2.1, in the sense that for generic initial conditions all trajectories converge to a point in this set.

- vi. For every X belonging to the attractor set, the set of nodes *i* for which  $X_i > 0$  is the same and is uniquely determined by *C*. The subgraph formed by this set of nodes will be called the "subgraph of the attractor" of Equation 2.1 for the graph *C*. Physically, this set consists of nodes that always end up with a nonzero relative population when the dynamic (Eq. 2.1) is allowed to run its course, starting from generic initial conditions.
- vii. If  $\lambda_1(C) > 0$ , the subgraph of the attractor of Equation 2.1 is an ACS. This ACS will be called the dominant ACS of the graph. The dominant ACS is independent of (generic) initial conditions and depends only on *C*.

Since Jain and Krishna's (2002) model is adopted in the study, we have also opted to take PFE as the attractor for our model. All the terminologies in this Section 2.5 formed the basis for the dynamic model.

# 2.4 Concluding Remarks

Through the reviewed literature, it is decided graph theory will be the basis of the model of the incineration process in which the Jain and Krishna's model (Jain and Krishna, 1998; 1999; 2001; 2002; 2003; Krishna, 2003) would be adopted along with some modifications in order to suit the system. Our understanding of all the concepts introduced in this chapter: graph theory, non-negative matrices, flow and multicommodity flow theory, autocatalytic sets and dynamics model; put us in a very good position to proceed with our formulation of the model of a clinical waste incineration process discussed in the consequent chapters.

# **CHAPTER III**

# GRAPHICAL MODELS REPRESENTING THE CLINICAL WASTE INCINERATION PROCESS

# 3.1 Introduction

Now we are ready to construct the model for the clinical waste incineration process based on our understanding of the theories studied and introduced in the previous chapter. We begin with the formulation of graphical models to represent the clinical waste incineration process. The knowledge of the incineration process explained in Section 2.2.1 has also helped to aggravate the development of these models. It starts with the development of a graphical model representing the connections between the parameters of the incineration plant. This model is considered as the basic model for the study and the details are discussed in Section 3.2. In doing so, we are actually trying to relate the input-output variables with the four components of the incinerator. Attempts to develop the flow model for the process has met some challenges and are described in Section 3.3.

The dynamic graphical model represent the incineration process is developed by selecting, modifying and enhancing the basic model and this is described in Section 3.4. The proposed graphical model is only a symbolic representation of the dynamic interaction between variables in the clinical waste incineration process. However, this model forms the focal point of the study and is anticipated to induce the subsequent research work, in particular to obtain a dynamic graphical model that is able to describe the dynamic nature of the incineration process as discussed in Section 3.5.

# **3.2** Construction of Graph Representing Flow of the Incineration Process

The study on original schematic diagram, the material balance chart for the plant and the operational data of measured variables along with the discussion on the flow of the process given in subsection 2.2.2.2 has enhanced our comprehension of the incineration process. For simplicity, the schematic diagram has been reconstructed (see Figure 2.4). By analyzing the reconstructed diagram and sorting out the elements in the data gives the pattern that was sought for. The abstraction of the problem has led us to look at the flow of the incinerator where we try to relate the various elements involve in the system.

Thus, we attempt to construct a graphical model explaining the connections between the parameters of the incineration plant. Here, the graph developed is to represent the relationship of the parameters in the plant. But, at the same time, we want this graph to be advanced enough to describe the relationship between the variables in the incineration process with the various components of the incinerator. This initiated the work in looking at the relationship of the parameters in the facility. Thus, it is deemed necessary to introduce symbols and assumptions to facilitate the construction of the graph.

#### **3.2.1** Symbols for Graph Representation

In the incineration plant, there are two categories involved (see schematic diagram, Figure 2.4), namely the incineration or combustion system and Air Pollution Control System (APCS). The incineration system consists of two components: the Primary Combustion Chamber (PCC) and Secondary Combustion

Chamber (SCC). We considered PCC, SCC and APCS as the physical components in the incineration plant.

What we want here is to find the relationship between the input-output variables of the process and the three physical components of the incinerator. We take these variables and the components as the parameters of the graphical model. We named the physical components as vertices of the graph, and they are symbolized as  $v_i$ , where:

- **v**<sub>1</sub>: Primary Combustion Chamber (PCC)
- v<sub>2</sub>: Secondary Combustion Chamber (SCC)
- v<sub>3</sub>: Air Pollution Control System (APCS)

The relations of the input-output variables are taken as links to the graph. They are denoted as edges  $(\mathbf{e}_i)$  with respect to each of the above components. We have identified a total of 20 edges and each of them is briefly discussed below.

The primary combustion chamber is preheated at a temperature of more than  $650^{0}$ C. This temperature is obtained by the burning of wood at 50 kg/hr for at least 72 hours. Here, the wood is considered as one that originated from the environment and it serves as an input for the primary chamber denoted here as  $e_1$ . The clinical wastes on the hand are the vital input for the incinerator and are noted as  $e_2$ . The wastes are collected from various government or private hospitals or clinic throughout the southern region. They are of heterogeneous mixture of general refuse, laboratory and pharmaceutical chemicals, containers, pathological wastes and cytotoxic wastes as presented in Table 2.1.

The primary chamber is a stepped hearth type consists of three stationary hearths on which the waste burns. Each zone of the hearth is equipped with modulating combustion air supply and independent ash pusher controls. This equipment allows total flexibility and permits the incinerator to operate efficiently as the properties of the waste may change in future. Here, the combustion air supply is named as  $e_3$ . As the waste is pushed through the incinerator, it progressively burns to

ash. The incinerator combustion ashes denoted as  $e_4$  are discharged from the primary chamber into water sealed trough for immediate quenching. These ashes are then removed from the trough by means of drag type ash conveyor.

Temperature control within the primary chamber is critical to prevent the melting and subsequent fusion of glass. Here, the temperature at the first and second hearths is denoted as  $\mathbf{e}_5$  and the temperature at the third hearth is denoted as  $\mathbf{e}_6$ . These are temperatures acquired within the primary chamber. The combustible gases produced can be considered to be a fuel and are mixed with air and completely combusted in the secondary chamber after ignition by a diesel burner in the ignition chamber (IPC Guidance Notes, 1996). The exhaust gases known as the product of combustion from the primary combustion ignition chamber and denoted as  $\mathbf{e}_7$ , is drawn into the secondary combustion chamber (SCC). Temperature exiting from the primary chamber and entering the secondary chamber is taken as  $\mathbf{e}_8$ .

This zone in SCC is equipped with auxiliary diesel fuel burners. An auxiliary fuel burner is used to maintain the secondary combustion chamber temperature. The fuel denoted as  $\mathbf{e_9}$  is injected into the secondary chamber along with the burner air supply which is denoted as  $\mathbf{e_{10}}$ . Combustion air denoted as  $\mathbf{e_{11}}$  is supplied by the secondary combustion air fan and is controlled to maintain an oxygen level of not less than 7%. The performance of the combustion process is monitored continuously using the flue gas analyzers, installed immediately outside the chamber.

The critical parameters when determining the efficiency of an incinerator secondary chamber are the combustion temperature, the chamber combustion time or residence time and the turbulence or contact time with excess air. This combustion temperature serves as an output for the secondary chamber and it is detected at the outlet of the secondary chamber and is taken as  $e_{12}$ . The incineration plant is installed with on line gas analyzers to continuously detect the emissions of Oxygen (O<sub>2</sub>), Carbon Monoxide (CO) and Carbon Dioxide (CO<sub>2</sub>) immediately outside the secondary combustion chamber. All of these gases play important role in indicating the performance of the incineration process. The combustion efficiency of the incineration process is determined by both the concentration of CO and CO<sub>2</sub> formed

in the combustion unit (Bruner, 1985). These gaseous are denoted respectively as  $\mathbf{e_{13}}$  and  $\mathbf{e_{14}}$ . While the O<sub>2</sub> gas is taken as  $\mathbf{e_{15}}$ . The O<sub>2</sub> level serves as an indicator of whether enough air is fed into the system for complete combustion. All of these gaseous are routinely recorded in the daily operation of the plant.

Besides these gases, there are also water particles (H<sub>2</sub>O) and other gaseous particulate that escaped the secondary chamber namely Nitrogen Oxide (N0<sub>2</sub>), Chlorine (Cl), Hydrogen Chloride (HCl) and Principal Organic Hazardous Constituent (POHC). Some of these POHC that are of concerned to the public are the dioxin and furan. All these gaseous particulate are grouped together as Pollutants and the Pollutants combined with H<sub>2</sub>O are taken as  $e_{16}$ . The plant ensures that its combustion performance is maintained at least 99% at all time. The O<sub>2</sub> level is activated once the combustion performance starts to decrease and that the level of O<sub>2</sub> is always maintained well above 11% level during the combustion process.

The products of the incineration process will enter the Air Pollution Control System (APCS). This system serves as a flue gas cleaning unit of the incineration facility. The flue gas that exited from the secondary chamber is first passed through a ceramic heat-exchanger unit before it is cooled further in a cooling tower (at the same time acts as a spray chamber) to a suitable temperature by atomizing water with compressed air. It then passed through a rotary contactor where lime and activated carbon absorbent are sprayed and mixed uniformly in the flue gas. From here, the gas passes through a cyclone, pulse-jet fabric filter, and wet scrubbing system before it is finally discharged into the atmosphere through a 20 meter high stack at the temperature of  $150^{0}$ C.

The flue gaseous discharged from the stack include  $O_2$ , CO,  $CO_2$  and  $H_2O$  along with Pollutants which are now in a cleaner state are brought back into the environment. These variables are noted consecutively as  $e_{17}$ ,  $e_{18}$ ,  $e_{19}$  and  $e_{20}$ . The whole process of the incinerator seems to be a cyclic in nature whereby the waste is being put in through the PCC (along with the help of combustion air) into the SCC (with the injection of fuel and air) into the APCS then back to the environment in the form of ashes and gas emission.

We made several attempts to develop the model using the parameters but none made sense. This is because the variables entering  $v_1$  have no source and those variables coming out of the  $v_3$  have no terminal point. Furthermore, we acknowledge that there must exist a source of these variable coming in to  $v_1$  and the gaseous resulted from the  $v_3$  must be eliminated from the system. Reflecting on the choice of parameters, we deduce that it is necessary to have the Environment as part of the physical component. This will be the fourth vertex of the graph, that is  $v_4$ . Thus, we have the list of components as below:

- **v**<sub>1</sub>: Primary Combustion Chamber (PCC)
- v<sub>2</sub>: Secondary Combustion Chamber (SCC)
- **v**<sub>3</sub>: Air Pollution Control System (APCS)
- v<sub>4</sub>: Environment

Our justification for the inclusion of environment is that the whole process of the incinerator is suppose to be cyclic in nature, in particular, the waste is being put into the system to be incinerated and as the result, the ashes and the cleaned air were brought back to the environment. This has actually make the resolution clearer and making more sense in representing the real connections between the parameters in the system. This brought us to the following result:

#### Result 1

In summary, we can group all the components and the input-output variable of the flow of the process into two distinct sets namely the set of vertices V and the set of edges E. These two sets are listed below:

$$V = \{ v_1, v_2, v_3, v_4 \}$$
 and

$$E = \{ e_1, e_2, e_3, e_4, \dots, e_{20} \}.$$

Now, we are ready to construct the graph.

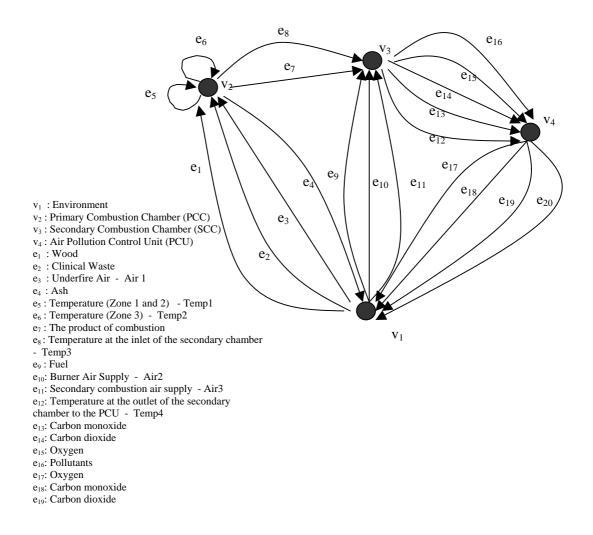
# 3.2.2 The graph

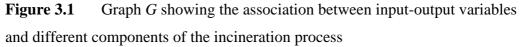
The observations, assumptions and the symbols introduced regarding the particular incineration plant in Malacca as discussed in the above Section 3.2.1, can be regarded as the proof by construction of the following proposition.

# **Proposition 3.1** (Sabariah et. al 2002b)

The incineration process of a clinical waste incineration plant in Malacca can be presented by a graph G(V, E): where a set V of vertices corresponds to the different components related to the incinerator and a set E of edges corresponds to the inputoutput variables associated with the components.

We identified the variables affecting the incineration process and clarified their relations to each other and their connections with respect to the different components in the incineration plant. Next is to translate the flow of the incineration plant to a graphical presentation. Translating the incineration system to a graphical model is to provide a fundamental abstraction of the system to a mathematical point of view. In other words, the concrete nature of the incineration plant is expected to be transformed into an abstract form. In this form, the flow of the system is clear and it also initiated our consequent modeling work. Therefore, graph G(V, E) in Proposition 3.1 is shown in Figure 3.1.





Graph G does provide a good representation of the connections between the parameters of the incineration plant. The visualization provided by the graph is indeed sufficient for us to comprehend the relationship of the parameters in the system. The graph theoretical concepts we have studied as introduced in the previous chapter has instigated us to explore further the features of this particular graph. This led to the following discussion on the properties of the graph.

# 4.3 Some Properties of the Graph

The study has successfully modeled the relationship of the input-output variables and the components of the incinerator in the form of a graph. One

interesting feature of the graph shown in Figure 3.1 is that the clinical incineration process is seen to originate from and back to the Environment. This corresponds to the worries aired by the public that argue incineration merely transfers pollutant from the solid media (waste) to the air (via stack emissions), water (via scrubber discharges) and ashes.

Through abstraction and reflection of the graph has led us to some of its properties that could further explain the relationship between the variables.

### 3.3.1 Eulerian

The first property to look at was to see whether the graph is Eulerian or not. To show this, the indegree and outdegree (refer to Definition 2.9) were obtained for each vertex of the graph as shown in Table 3.1.

**Table 3.1**:
 Indegree and Outdegree for each vertex

	$V_1$	<b>V</b> <sub>2</sub>	<b>V</b> <sub>3</sub>	$V_4$	Total
Indegree	5	5	5	5	20
Outdegree	6	5	5	4	20

# Result 2

It is not easy to get an Euler circuit that is a circuit passing through each vertex at least once and traverses every edge of G exactly once. Clearly, from Definition 2.9 and Table 3.1, it could be seen that the graph does not have an Euler circuit. This actually has no significant impact on the study since the edges represent the input-output variables and all of them not necessarily can be traverse in a single path.

### Result 3

Nevertheless, the graph does contain Eulerian trails from  $v_1$  to  $v_4$  (Definition 2.9) as documented by Wan Rukaida (2003). Table 4.1 shows the following:

od  $v_1 = in v_1 + 1$ ,  $in v_4 = od v_4 + 1$  and  $od v_2 = in v_2$ ,  $od v_3 = in v_3$ .

#### **Physical Interpretation of Result 3**

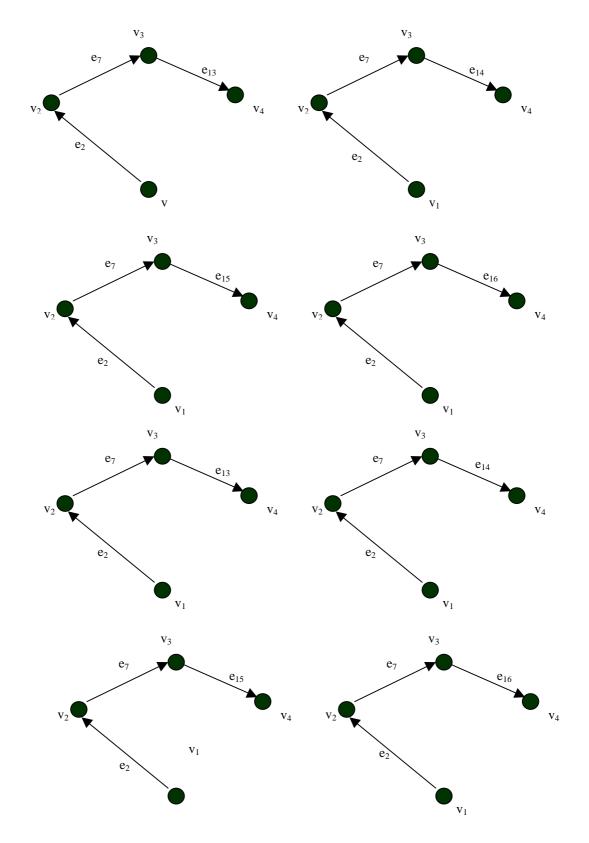
This indicates that the graph has Eulerian trail from  $v_1$  to  $v_4$ . An interesting explanation to these endpoints of the trail was that the processes in the system (incineration process and the cleaning of the gaseous produced during incineration) actually starts at  $v_1$  and ends at  $v_4$ . Completing the process, all the gaseous is brought back to the atmosphere through the stack (in other word they are brought back to the Environment). Therefore, the Eulerian trail from  $v_1$  to  $v_4$  shows the trail of the input-output variables during both processes of the system.

#### Result 4

There is a combination of 30 Eulerian trails constituting the sub-graphs of the graph G. Since waste is the most crucial input of the incinerator and in fact is vital to the existence of the incineration plant, the following trails (see Figure 3.2) are deemed to be important in describing the flow of the waste in the incinerator.

#### **Physical Interpretation of Result 4**

The trails explained the decomposition of the waste into different products in the incineration process that begin in the loading of waste obtained from the surrounding area of the incinerator plant  $(v_1)$  to the primary chamber  $(v_2)$  where it was being burnt to produce the product of combustion. This product of combustion was then further combusted in the secondary chamber  $(v_3)$  to produce other gaseous which in turn proceed to the Air Pollution Control System  $(v_4)$  to be cleansed as shown in the trails in Figure 3.2.



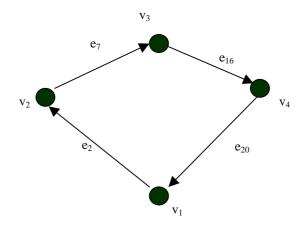
**Figure 3.2** Eulerian trails describing the flow of waste in the incineration process

# 3.3.2 Hamiltonian

Reflecting on the schematic diagram of the incinerator plant shown in Figure 2.4, has made us understand that each of the variables entering the PCC has to go through each consequent component to the atmosphere in the form of gaseous. Thus, what is important here is that the path taken by these variables must go through all the vertices. This brought the study to the investigation of the next property of the graph that is whether the graph is Hamiltonian or not.

# Result 5

From the definition and the proposition on Hamiltonian (Definition 2.10), we could see that the graph is Hamiltonian. We could obtain several Hamiltonian circuits for the graph. An example of the Hamiltonian circuit H for the graph is shown in Figure 3.3.



**Figure 3.3** A Hamiltonian circuit *H* for graph *G*.

# **Physical Interpretation of Result 5**

Beside representing the connections of the variables in the incinerator plant, the Hamiltonian circuits or subgraphs of this graph can also represent the chemical reaction taking place in the incinerator. An example of this visualization by Hamiltonian subgraph H, is given by a particular circuit given concretely as

*H*: 
$$v_1 e_2 v_2 e_7 v_3 e_{16} v_4 e_{20} v_{11}$$

We can interpret this path of Hamiltonian subgraph as the product of chemical reaction of a clinical waste of heterogeneous mixture being put into the PCC. The wastes incinerated in the chamber would result in the products of combustion. These products of combustion entered the SCC and further combusted there to form various gaseous particulates (N0<sub>2</sub>, Cl, HCl and POHC) and water particles, grouped together as the combination of H<sub>2</sub>O and Pollutants. These pollutants are the products of the wastes characterized in Table 2.1. The gases had to undergo the process of cleansing in the APCS and the cleaner gases passed through the stack back into the environment. The same kind of explanation is when wood made an input to the PCC instead of the wastes and when we took the other gaseous instead of the pollutants.

In fact, the Hamiltonian subgraphs in this problem are suitable in representing the product of the combustion of wood and waste. For instance, if the emphasis is given to what happen to the waste being burned in the process, then the edges (the variables) corresponding to the product of burning of waste would seem relevant and can be interpreted well by the circuit. Otherwise, the circuit would not give a good interpretation of the result of the burning of waste taking place in the incinerator. Such example would be the following circuit:

$$H: v_1 e_2 v_2 e_8 v_3 e_{13} v_4 e_{20} v_1$$

Here, the temperature  $e_8$  might explain for the result of the waste burning, but carbon monoxide would not result from the temperature and the same would account for H<sub>2</sub>O and pollutants after  $v_4$ . Therefore, we could only select certain subgraphs in order to describe the reactions especially in looking at the changes in the waste and the wood.

# Result 6

The connections of the variables in the incinerator plant, shown in Figure 3.2 and Figure 3.3, signifying both properties are almost similar. The difference between Eulerian trails and the Hamiltonian subgraphs of the graph G was that the former described the flow in the incineration process whereas the later explained the flow of the whole system of the incinerator. The trails are in fact sufficient in showing the

outcome of the system since the variables coming out of the APCS were actually the same gases, the difference would only be on their quantity. This is because the gaseous coming out of the APCS is cleaner and reduced in its amount than the ones entering the system.

Graph G as an abstraction of the system to the mathematical form is seen to be a very potential manipulative structure in which we could derive some description or further explanation about the system. We are seeking a way or a method on how the graph G be used to attain our goal of the study, that is, to model the incineration process. The similarity in the 'flow' concept of graph G and the flow model theory observed through the process of comparing and contrasting between what we have discussed so far in this section to the works in flow theory (Ahuja et al., 1993), a natural shift was to look at the problem in the direction of the flow theory. This has further motivated the study to indulge in the flow model.

### 3.4 Flow Model

The association of input-output variables with respect to the different components of the clinical waste incineration process has successfully modeled by graph G. This result serves as a basis for the understanding of the whole process of the incinerator and in exploring the unique relationship between the underlying variables in each of the components. By comparing the similarity between the Eulerian trails discussed in the previous section and flow theory, has induced the problem to network flow modeling.

Basic questions commonly addressed by network flow problems are shortest path problem, maximum flow problem and minimum cost flow problem. In this study, at the beginning of the problem, we were interested to see how we could maximize the performance of the process. At this juncture, flow model seems appropriate and worth investigating further since we know that flow model has capacity in many applications. We introduced two subgraphs for the graph G namely subgraph (a) and subgraph (b) in Figure 3.4 to represent the material flow and the temperature flow of the whole system, respectively. The introduction of these subgraphs actually specialize our problem into a particular case.

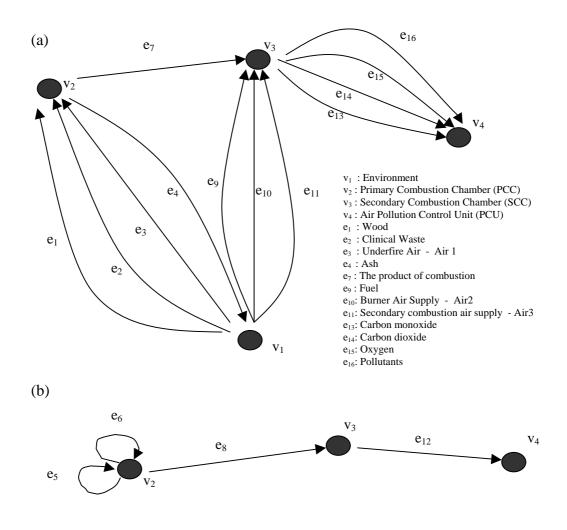


Figure 3.4 (a) Subgraph representing the material flow and(b) Subgraph representing the temperature flow of the incineration process

These subgraphs were initiated by considering the endpoints of the Eulerian trails of *G* (see Result 3). Here,  $v_1$  was chosen as the source and  $v_4$  as the sink of the network. This explained the fact that the incineration process begins at  $v_1$  and ends at  $v_4$ . To describe the incineration process and to achieve the objective of optimizing the process, the subgraph (a) representing the material flow was considered. The consideration of waste as the vital input to the incinerator and also the emphasis on understanding the changes of the materials (variables) in the process, has further confirmed our choice of using subgraphs (a) in Figure 3.4 and more specific the

Eulerian trails in Figure 3.2 to be considered in the flow modeling of the clinical waste incineration process.

# Result 7

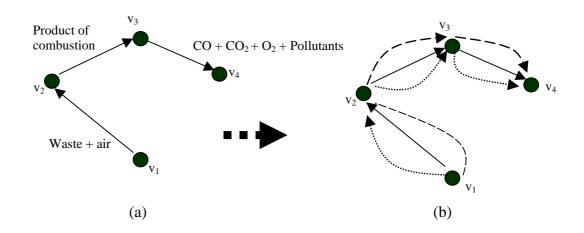
Even though the Eulerian trails fitted perfectly in describing the source and the sink of the network and seems relevant to indulge the study into the field of flow theory, but the explanation or the logic of the flow could not be satisfied by the subgraph. In general, the flow theory is the study of flow of variables in a network. This means that whatever variable going in to any vertex must be the same variable that was coming out of it. The trails prescribed as in Figure 3.2 did not match this condition due to the chemical reactions taking place in the incineration process. This situation prompted us to do further investigation and simplification if we want to extend the work in the network flow theory. Further specialization, that is, by considering the relationship and properties of graph G has brought this research to a particular branch of network flow theory known as multicommodity flow.

# 3.4.1 Multicommodity Flow Modeling

The flow model explained by the subgraph 3.4(a) leads to the study of multicommodity flow problems. Multicommodity flow problems arise when several commodities use the same underlying network. The commodities may either differentiated by their physical characteristics or simply by their origin – destination pairs. Many large scaled models are formulated as multicommodity flow problems. This model arises in a wide variety of application settings such as communications, logistic, manufacturing and transportation.

# Result 8

The variables represented by the edges are considered the multicommodities of the network since they satisfy the condition stated above. At every vertex the nature of each commodity changes and this prompted the investigation of each eulerian trails of the graph (see Figure 3.2). With the assumptions that wood is not playing a great role in the combustion except as start-up fuel and that the incineration process is of 100% perfect burning left the work with the four Eulerian trails beginning at  $v_1$  and ends at  $v_4$  as given in Figure 3.2. These Eulerian trails were further integrated to form a single multicommodity flow model that would serve as a basis in describing the incineration process shown in the following Figure 3.5.



**Figure 3.5** Multicommodity flow showing the flow of different variables in the incineration process

### **Physical Interpretation of Result 8**

The flow model (b) of Figure 3.5 shows the flow of the multicommodities in the incineration process. These commodities comprise of the chemical components and hence the problems be based on the chemical flow in the clinical waste incineration process. A possible answer to this problem is to break down the clinical waste into its chemical components such as carbon, hydrogen, chlorine, oxygen and so on. Then the graph (b) of Figure 3.5 would be able to represent the flow of each of this chemical component throughout the process. However, following through this idea has brought up some new challenges.

### 3.4.2 Set Back of the Multicommodity Flow Model

The work on this multicommodity flow problem met its challenges when these two decisions were taken into account.

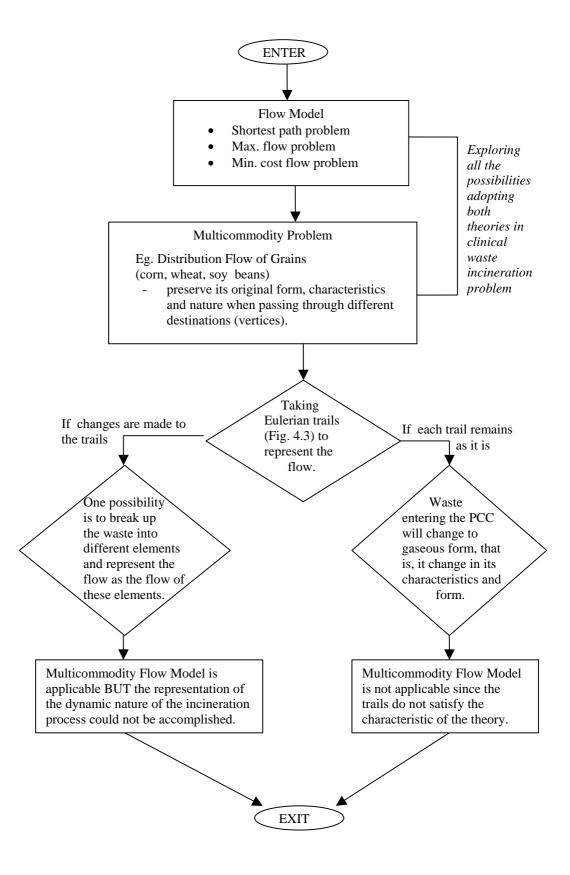
#### **Decision 1**

To enable the study to indulge further in the realm of multicommodity flow problem, all of the variables have to be broken down into different chemical components. The breaking down of wastes into their respective chemical components gave the most difficulties since the waste are of heterogeneous type (Bruner, 1985). The chemical components that constitute different type of waste are again could be of different family of chemical bonding such as containers and plastics made of Polyvinyl chloride (PVC). Even, the waste from the pathological laboratories also could be varied range in nature and chemical constituents. These complicate the study even further and the description of the flow model would not be precise enough with all these uncertainties.

### **Decision 2**

The other set back is that this flow model does not really present the real process of the incinerator. Even though the effort can be continued, that is the flow of the elements comprised in the waste and the air, can be represented by the flow model but the dynamic of the process could not be ascertained by this type of flow model. This is due to the existence of the components in the incinerator plants namely  $v_1$ ,  $v_2$ ,  $v_3$  and  $v_4$ . The flow would then be just like the flow of any fluid or gaseous materials in a piped line, and does not give any indication of the interaction of the chemicals in the incineration process.

Figure 3.6 summarizes our attempt to summon the problem in the theory of flow model. The diagram indicates that we have to end the exploration in flow theory not because of the infeasibility of the theory. It is due to the difficulty in breaking up of components in the waste. Even though it is possible to do it, the presentation would not signify the real process of the clinical waste incinerator.



**Figure 3.6** Summary of our attempt in the theory of flow model in extending the clinical incineration process

## 3.5 The Dynamic Graphical Model

The dynamic nature of the clinical waste incineration process would not be presented using graph G nor embarking in the flow modeling theory based on the graph. Nevertheless, graph G initiated the evolution of another graphical representation of the process explaining its dynamical aspects. We are able to put ourselves back on the track of solving the problem in graph theoretical concept. We began specializing by looking only at the input-output variables in the incineration process.

#### **Decision 3**

The four components of the incinerator plant were discarded from graph G when we consider that the emphasis of the study was to investigate the role played by the variables in the incineration process and not on exactly where it happen. In this regard, the process was assumed to be taking place in one compartment (the incinerator). The variables were naturally taken as the vertices and edges are the directed links between these variables. Beginning with this specialization process in which the assumption of the process happening in one particular chamber (in which, the four components were omitted), we made further assumptions and is discussed next.

The number of variables considered in the new graph has decreased due to the following reasons and assumptions:

- (a) There are repetitions on some of the variables, due to the location of their existence, in the graph G.
- (b) All the temperatures are also disregarded because we assumed that the temperature was controlled in the process. The study on the year 1999 data done by Nor Hidayati (2001) in analyzing the relationship between the waste weight and the temperatures of the chambers has found that the incinerator plant was operating within the set temperatures of  $900^{\circ}$  to  $1000^{\circ}$ C in the primary chamber and  $1000^{\circ}$  to  $1100^{\circ}$ C in the secondary chamber.

- (c) Ashes were removed here with the assumption that it is still considered as part of the waste being leftover as the result of the incineration process.
- (d) Wood was also omitted here with the assumption that it was only used during the start-up period. In this case, it was assumed that the process taking place whenever the compartment (the incinerator) was in a stable condition or in an operation condition.

#### **Decision 4**

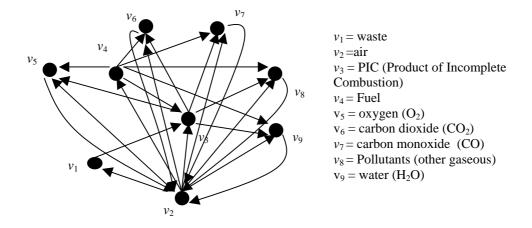
Taking into account all the above considerations and assumptions, the number of variables taken decreased from 20 to 9. Several graphs were then studied to see their relevancy in representing the process. The rationale of each phase of the selection of graphical model is presented based on the selection of vertices as well as the selection of the links for the graph. Several other graphs were actually evaluated in the study but those presented below were among the few examples investigated. It started from nine variables network and eventually reduced to the one with six variables. In the light to attain the most appropriate network to represent the dynamics of the incineration process, each graph was reviewed and was further refined. Consequently, our discussion will be on the selection of the vertices in Section 3.6.1 and the illustration on the selection of edges in Section 3.6.2. Both these selections were based on the knowledge in chemistry.

# 3.5.1 Refinement of Vertices for the Network

By making the above assumptions, we began looking at the refinement of the vertices of the graph. We begin looking at the graph having nine variables as shown in Figure 3.7.

#### Result 9

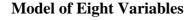
## **Model of Nine Variables**



**Figure 3.7** Graph with nine variables in representing the dynamics of the system

Here, nine variables are considered. This graph was further simplified because of the temporary state of the Product of Incomplete Combustions (PIC). The PIC was the intermediary product in the burning process and in fact will eventually result in the formation of other gaseous. We decided that this PIC be removed from the model. The model was then reduced to only 8 variables.

### Result 10



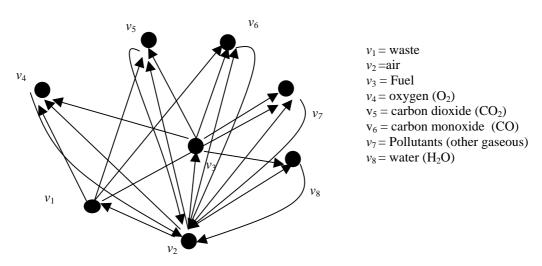


Figure 3.8 Graph with eight variables in representing the dynamics of the system

Omitting the PIC has resulted in the consideration of the above model shown as in Figure 3.8. Here again, the model was being *reviewed* to see its relevancy to the system. Looking at the redundancy in noting both air and oxygen, we decided to omit air from the model. The *air* comprise of oxygen and nitrogen. But in the actual combustion, the gas that was really consumed in the process was oxygen. This has led the study to discard the air with the assumption that it was equitable to oxygen. With this omission, a model with seven variables was then considered.

#### Result 11

#### **Model of Seven Variables**

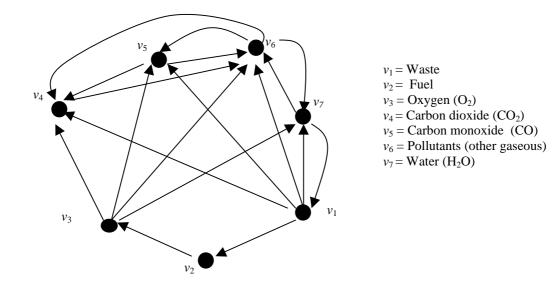


Figure 3.9 Graph with seven variables in representing the dynamics of the system

Figure 3.9 shows the model of seven variables for the clinical waste incineration process. Reviewing this model has again resulted in another refinement of the model. Here, Pollutants (other gaseous than  $CO_2$  and CO) and Water (H<sub>2</sub>O) are combined and represented as one single variable. As stated earlier in the chapter, the combustion efficiency of the incineration process is determined by the presence of  $CO_2$  and CO at the end of the process. This has prompted the study to concentrate on these two gases and decided to group together the variables H<sub>2</sub>O and Other Pollutants as one. Joining these two variables together has brought the study to consider several models of six variables in which they were then scrutinized to produce a final graph chosen to represent the clinical waste incineration process.

#### Result 12

## **Model of Six Variables**

Several models of six variables shown as in Figure 3.10 are further considered in the study to represent the clinical waste incineration process. Even though they are of the same number of vertices but slight change in positioning the edges has resulted in different graph representation. At this stage, the six variables considered are seen to appropriately and sufficiently representing the vital parameters in the process. The only thing to look into now was whether the positioning of the edges was correct. Hence, this has prompted the study to make further reflection and reviewing of each of these models in order to finally deciding on a single model best fit for the process.

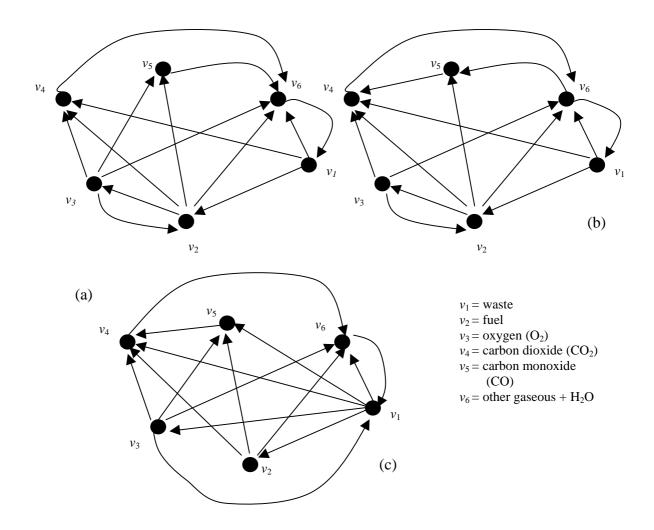


Figure 3.10 Models of six variables in representing the dynamics of the system

On examining the graphs and evaluating the relationship of these variables in term of the chemical reaction taken place in the incineration process, the graph Gshown in Figure 3.10c, called  $G_d$  was chosen. The vertices of the graph correspond to the variables and a directed link from vertex j to vertex i indicates that variable jcatalyzes the production of variable i. So far, we have discussed the rationale of choosing six variables representing the system. Next, we discussed the rationale made in choosing the links of this particular network and would therefore justified the reason why we chose Figure 3.10(c) to represent our dynamic graphical model.

#### **3.5.2** Refinement of Links for the Network

We have discussed in the previous subsection on how we derived the number of vertices seen appropriate for the system. This subsection will help us to understand the reason of our refinement of the links (edges) for the graph  $G_d$ . Before we proceed, let us first summed up about the graphical model, graph  $G_d$ .

### Result 13

The model  $G_d(V, E)$  consists of:

(a) Six vertices represent the six variables or species that play vital roles in the clinical waste incineration process, namely Waste, Fuel, Oxygen, Carbon Dioxide, Carbon Monoxide and Other Gases including Water.

 $V = \{v_1, v_2, v_3, v_4, v_5, v_6\}$  is the set of vertices for the network,

where 
$$v_1 = Waste$$
  
 $v_2 = Fuel$   
 $v_3 = Oxygen (O_2)$   
 $v_4 = Carbon Dioxide (CO_2)$   
 $v_5 = Carbon Monoxide (CO)$   
 $v_6 = Water (H_2O) + Pollutants$ 

(b) Fifteen edges representing the links of the variables in the process due to their catalytic relationship and is denoted by the set E.

$$E = \{(v_1, v_2), (v_1, v_3), (v_1, v_4), (v_1, v_5), (v_1, v_6), (v_2, v_4), (v_2, v_5), (v_2, v_6), (v_3, v_1), (v_3, v_4), (v_3, v_5), (v_3, v_6), (v_4, v_6), (v_5, v_4), (v_6, v_1)\}$$

where

- $(v_1, v_2)$ : 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 (1992) is O<sub>2</sub>. This means that waste is contributing a certain amount of O<sub>2</sub> to the chamber. In fact, the initial amount of O<sub>2</sub> in the chamber taken as the concentration dynamics of this variable in Chapter 6 actually relates to this interaction.
- ( $v_1, v_4$ ): CO<sub>2</sub> is the product of combustion of waste. Consequently, waste catalyzed the production of CO<sub>2</sub>. This can be seen from the following simple chemical reaction equation between C (carbon) present in the waste and also O<sub>2</sub> (Bruner, 1991)

$$C + O_2 \rightarrow CO_2$$

( $v_1$ ,  $v_5$ ): CO is also the product of combustion of waste. This gas is produced as a result of an insufficient amount of O<sub>2</sub> in the chamber. This could be seen from the equation below:

$$C + \frac{1}{2}O_2 \rightarrow CO$$

 $(v_1, v_6)$ : H<sub>2</sub>O and Pollutants are the products of combustion of waste. Therefore, waste catalyzed the production of these variables. Almost by its very definition, waste is not able to be classified into a single, or even multiple, known chemical structure. Often the chemical nature of a particular waste is unknown. Therefore, the following assumptions were made in considering the relation between these two variables (Bruner, 1991).

• All hydrogen present converts to water vapor, H<sub>2</sub>O.

 $2H_2 + O_2 \rightarrow 2H_2O.$ 

- All chloride (or fluoride) converts to hydrogen chloride, HCl (or hydrogen fluoride, HF.
- All sulfur converts to sulfur dioxide, SO<sub>2</sub>.
- Alkaline metals converts to hydroxides: sodium to sodium hydroxide (2Na + O<sub>2</sub> + H<sub>2</sub> → 2NaOH) and potassium to potassium hydroxide (2K + O<sub>2</sub> + H<sub>2</sub> → 2KOH).
- Nonalkaline metals convert to oxides: copper to copper oxide (2Cu + O<sub>2</sub> → 2CuO), iron to iron oxide (4Fe+ 3O<sub>2</sub> → 2Fe<sub>2</sub>O<sub>3</sub>).
- ( $v_2$ ,  $v_4$ ): In the waste and fuels normally encountered, the major constituents include carbon and hydrogen. For an equilibrium equation for a simple fuel, methane CH<sub>4</sub>, we have CH<sub>4</sub> + 2O<sub>2</sub>  $\rightarrow$  CO<sub>2</sub> + 2H<sub>2</sub>O. From this equation, we can conclude that the fuel (diesel) used in the chamber must also contribute to the production of CO<sub>2</sub>.
- $(v_2, v_5)$ : In the case, where O<sub>2</sub> is insufficient, there is possible production of CO in the chamber. This can be explained by the following equation (Bruner, 1991).

 $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O + CO$  (trace)

Even though a trace of CO is being produced, nevertheless, this equation shows that fuel catalyze the production of CO.

- ( $v_2, v_6$ ): The equation CH<sub>4</sub> + 2O<sub>2</sub>  $\rightarrow$  CO<sub>2</sub> + 2H<sub>2</sub>O also shows that water is catalyzed by fuel.
- $(v_3, v_1)$ : 11% of waste constitutes of O<sub>2</sub> (Green, 1992). This means that O<sub>2</sub> is part of the waste especially at its initial stage in the chamber.

- ( $v_3, v_4$ ): C + O<sub>2</sub>  $\rightarrow$  CO<sub>2</sub> and CH<sub>4</sub> + 2O<sub>2</sub>  $\rightarrow$  CO<sub>2</sub> + 2H<sub>2</sub>O are examples of equations showing that O<sub>2</sub> is catalyzing the formation of CO<sub>2</sub>.
- ( $v_3, v_5$ ): The equation  $C + \frac{1}{2}O_2 \rightarrow CO$  explained the link between these two variables. It shows that  $O_2$  is the variable that motivates the formation of CO. Carbon monoxide, CO, is produced where insufficient oxygen is provided to completely combust a fuel. It is, therefore, indicative of burning, or combustion efficiency. The greater the amount of air presents and the greater the degree of turbulence, the less carbon monoxide will be formed. Thus, existence of CO must be considered and one of the sources of its existence is  $O_2$ .
- ( $v_3, v_6$ ): The equations showing the reactions between  $O_2$  and other molecules presence in waste and also fuel such as CH4 +  $2O_2 \rightarrow CO_2 + 2H_2O$ ,  $2Na + O_2 + H_2 \rightarrow 2NaOH$ ,  $2Cu + O_2 \rightarrow 2CuO$ ,  $4Fe+ 3O_2 \rightarrow 2Fe_2O_3$ and  $2K + O_2 + H_2 \rightarrow 2KOH$  indicates that  $v_3$  play a role in catalyzing  $v_6$ .
- ( $v_4, v_6$ ): CO<sub>2</sub> is actually a stable gas. But there are circumstances whereby, it will react with for example water vapor in the chamber to produce carbonic acid which we classified it as  $v_6$ . With this consideration given, we have the link  $v_4 \rightarrow v_6$ .

 $(v_5, v_4)$ : CO can react with O<sub>2</sub> to form CO<sub>2</sub> as shown by the following equation:

 $\text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2$ 

This reaction took place when excess amount of  $O_2$  is in the chamber. In actual process, this reaction seldom happen. 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  $CO_2$ . The link from  $v_5$  to  $v_4$  can exists since we have considered the formation of CO in the chamber, with enough amount of oxygen in the chamber.

( $v_6$ ,  $v_1$ ): About 23% of waste constitutes of water (H<sub>2</sub>O) as shown by Green (1992) and this explained the link from  $v_6$  to  $v_1$ .

Thus, through the above considerations and observations on the refinements of vertices and edges of the graph we come to the following proposition.

#### **Proposition 3.2**: (Sabariah et al. 2003)

The dynamic of the incineration process of the clinical waste incineration plant in Malacca could be presented by the graph  $G_d$  as in Figure 3.10c.

The focus of the rest of the study and the development of the model in describing the changes of the variables in the incineration process would be on this particular graphical model.

### 3.6 Concluding Remarks

This chapter illustrated several different graphical models representing the clinical waste incineration process. Even though each of them represents the same system, it connotes to the different interpretation depending on what we want from the system. Beginning with the graph representing the relations between the parameters in the incinerator plant, the study had proceeded with the attempt on extending the work in flow model. The challenges in pursuing the flow model had confronted us to take another approach to solve the problem. Nevertheless, the graph has shown to be the starting point for our consequent work to obtain a graph showing the dynamic of the system that is the derivation of the dynamic graph  $G_d$  (Figure 3.10c). Researching through the literatures has brought the study to the model of Jain and Krishna (2002) which in turn initiated the extension of this work. The model based on graph  $G_d$  (Figure 3.10c), would be discussed next in Chapter 4.

# **CHAPTER IV**

### AUTOCATALYTIC SET: BASIS FOR MODEL CONSTRUCTION

## 4.1 Introduction

The graph  $G_d$  (Figure 3.10c) representing the dynamic of the clinical waste incineration process developed in the proceeding chapter is scrutinized further in this chapter. Our aim now is to use this dynamic graphical model to develop a model that would describe the changes of the variables in the process and also the changes of the graph. Model proposed by Jain and Krishna (as described in Section 2.2.3) and our work so far are based on similar graph-theoretical concept. This actually advances our work further by adopting their model.

This chapter discusses the construction of the model, the key feature of which is the concept of Autocatalytic Set (ACS). With this note, the chapter begins with the discussion on the relationship of the notion of 'autocatalytic set', which play an important role in the dynamics of the model studied in this thesis, to the graph and also to the Perron-Frobenius eigenvectors of the graph (Section 4.2). The discussion then proceeds to the development of the model in which we obtained by adopting and modifying Jain and Krishna's model in Section 4.3. The implementation of the model to the clinical waste incineration process together with the analysis and suggestions pertaining to the results are highlighted in Section 4.4.

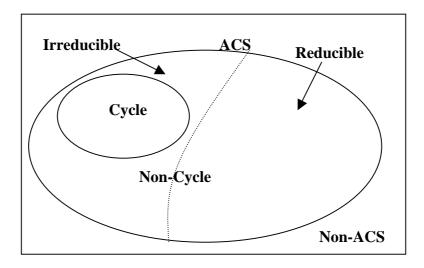
# 4.2 The Graph *G*<sub>d</sub> and Autocatalytic Set (ACS)

In this section we discuss the relationship between the concept of ACS and the graph. We studied all definitions and propositions proposed by Jain and Krishna regarding their modeling works to *abstract* some ideas and to obtain further *insights* on looking at our problem, specifically the graph  $G_d$ . Therefore, by this abstraction, we hope to extend our understanding and knowledge of the graph especially in its representation of the system and its relation to the model we were pursuing. Using Definition 2.17 and Proposition 2.2, we come to the following theorem:

## Theorem 4.1:

The graph  $G_d$  is an autocatalytic set.

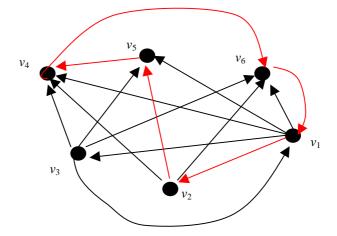
This theorem brought the graph closer to the notion of ACS and to the model of evolution proposed by the two researchers. In reviewing Proposition 2.3 has led us to the construction of the following Venn diagram in Figure 4.1 as a summary to the relationship between the concept of an ACS, cycle and irreducibility of a graph. This helps us to visualize these relationships better.



**Figure 4.1** Venn diagram showing relationship between cycle, irreducible and ACS

#### Result 14

Graph  $G_d$  contains a cycle but  $G_d$  itself is not a cycle. An example of a cycle of the graph is given in Figure 4.2 where it shows there is a path between  $v_1$ ,  $v_2$ ,  $v_5$ ,  $v_4$  and  $v_6$ . There exist other cycles that involved at most five nodes but none could be found to contain a path that passes through all the six nodes.



**Figure 4.2** A closed path in the graph *G* 

Since graph  $G_d$  is not a cycle, the Proposition 2.3(i) does not hold for the graph. The relation of graph  $G_d$  with Proposition 2.3(ii) will be interpreted when the irreducibility of the graph is discussed in the Section 4.2.2.

### 4.2.1 The Adjacency Matrix

The network of interactions between the variables in the clinical waste incineration process shown in Figure 3.11c can also be specified using the 6 x 6 matrix *C* called the adjacency matrix. The rows and columns of the matrices represent the nodes of the graph and the entries  $C_{ij}$  represent the link between the  $j^{\text{th}}$  node and  $i^{\text{th}}$  node. A directed weighted link from node *j* to node *i* is denoted by the following values.

$$C_{ij} = \begin{cases} 1 & \text{if there exist a link from } j \text{ to } i \\ 0 & \text{if there is no link from } j \text{ to } i \end{cases}$$
(4.1)

This gives the following adjacency matrix C

$$C_{ij} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \end{pmatrix}$$
(4.2)

Note that the adjacency matrix is the transpose of the usual one. This convention was chosen because it is more natural in the context of a dynamical system (Jain and Krishna, 1998; 1999; 2001; 2002; 2003; Krishna, 2003). In chemical process this situation was interpreted as *j* being a catalyst for the production of *i*. As can be seen here, self-catalytic process has been excluded by letting  $C_{ii} = 0$ .

The terms 'graph' and 'adjacency matrix' are interchangeable, both representing the same network of the system. From now on the phrase 'a graph  $G_d$  with adjacency matrix C' will be abbreviated to only 'a graph C'. An interesting feature denoted by the adjacency matrix (Equation 4.2) in looking and showing the autocatalytic set of the graph is that every row must contain at least one non-zero element. Any *i*<sup>th</sup> element represented by the *i*<sup>th</sup> row must be catalyzed by at least one other element of the *j*<sup>th</sup> column. This relate to the ACS of the graph whereby any node can have at least one incoming link from any other nodes in the graph. All the elements of the principle diagonal are zeros showing that there is no self-replicating of any of the elements.

Thus, by relating the concept of ACS through Definition 2.18 to the adjacency matrix of the graph, the following theorem was formulated:

#### Theorem 4.2:

*C* is an autocatalytic set iff for each i = 1, 2, ..., n there exist a  $j \neq i$ , j = 1, 2, ..., i - 1, i + 1, ..., n such that  $c_{ij} \neq 0$ .

### Proof:

(⇒) Suppose *C* is an autocatalytic set, therefore by Definition 2.17, each node has at least one incoming link. Now if *C* has *n* nodes, then *C* is  $n \times n$  matrix whereby each element of the *i*<sup>th</sup> row represents the link from any node of the set to the *i*<sup>th</sup> node. Since *C* is autocatalytic set, therefore  $c_{ij} \neq 0$  for each i = 1, 2, ..., n,  $\exists j \neq i$ , j = 1, 2, ..., i - 1, i + 1, ..., n.

( $\Leftarrow$ ) Suppose for each i = 1, 2, ..., n,  $\exists j \neq i$ , j = 1, 2, ..., i - 1, i + 1, ..., n,  $c_{ij} \neq 0$ . This means that the  $i^{th}$  node must have at least one incoming edge, therefore *C* has to be an ACS using Definition 2.17.

From this matrix, further investigations on the properties of ACS of the graph C were carried out. Since the adjacency matrix C is a non-negative matrix, we can relate it to Perron Frobenius Theorem (will be discussed in Section 4.2.2). Through this relationship, the characteristic of the graph can be determined by looking at the eigenvalues and the eigenvectors of it. Here, the eigenvalues  $\lambda$  and their respective eigenvectors **x**, were found using MATLAB version 6.1 as the followings:

$$\lambda = 2.08541, -0.10143 + 0.93936 i, -0.10143 - 0.93936 i, -0.94127 + 0.43399 i, -0.94127 - 0.43399 i, -0.00000$$
(4.3)

It should be noted here that the value -0.00000 given in Equation 4.3 as one of the eigenvalues is not exactly equal to zero. It has a value, but a very small one.

$$x = \begin{pmatrix} 0.38200\\ 0.18318\\ 0.18318\\ 0.53093\\ 0.35885\\ 0.61344 \end{pmatrix}, \begin{pmatrix} 0.16713 + 0.12095i\\ 0.10828 - 0.18961i\\ 0.10828 - 0.18961i\\ 0.10828 - 0.18961i\\ 0.10828 + 0.18961i\\ 0.067352\\ -0.31537 + 0.37440i\\ -0.23884 + 0.33433i \end{pmatrix}, (4.4)$$

$$\begin{pmatrix} -0.14106 + 0.42893i\\ 0.29686 - 0.31882i\\ 0.29686 - 0.31882i\\ 0.29686 - 0.31882i\\ 0.29686 - 0.31882i\\ 0.29686 + 0.31882i\\ -0.05957 - 0.19427i\\ -0.48090\\ -0.35024 - 0.14614i \end{pmatrix}, (4.4)$$

## 4.2.2 Relationship of an ACS to Perron-Frobenius Theorem

In this section, we relate the ACS of the graph to Perron Frobenius Theorem discussed in Section 2.3.2.2. We begin looking at the irreducibility of the graph. In this case, n = 6 gives

$$\left(I_6 + C\right)^5 = \begin{pmatrix} 23 & 23 & 22 & 5 & 1 & 12 \\ 40 & 41 & 40 & 12 & 5 & 23 \\ 53 & 57 & 54 & 18 & 11 & 33 \\ 97 & 103 & 97 & 30 & 16 & 58 \\ 75 & 80 & 75 & 23 & 13 & 45 \\ 108 & 115 & 108 & 33 & 18 & 65 \end{pmatrix}$$
(4.5)

where  $I_6$  is the identity matrix of  $6 \times 6$ .

# Result 15

Since all the entries of the matrix in Equation 4.5 are non-zero and using the Definition 2.13, it can be deduced that the matrix C is an irreducible matrix. An irreducible graph is always an ACS (the second part of Proposition 2.3(i)). Therefore, it supports the Theorem 4.1, that is, since graph C is irreducible graph

hence it is an ACS. It is an ACS and is irreducible, yet it is not a cycle. This relates to the second part of Proposition 2.3(ii).

## **Physical Interpretation of Result 15**

There are two connotations of the irreducibility concept of this matrix *C*. They are as follows:

- (i) Firstly, irreducibility as referred to the graph means that the graph is
   "strongly connected" (Epp, 1993), that is, it is possible to travel from one
   node to any other node strictly along the one-way paths in graph.
- Secondly, as referred to the dynamical system, saying that the matrix C is irreducible means that the system cannot be reduced. In other words, the system must be treated as a whole in studying its behavior.

## Result 16

For any non-negative irreducible matrix, the PF theorem (Section 2.3.2.2.1) guarantees that there exists an eigenvalue, which is real and larger than or equal to all other eigenvalues in magnitude. This largest eigenvalue is called the PF eigenvalue of the matrix, which we denote by  $\lambda_1(C)$  for the graph *C*. Here,

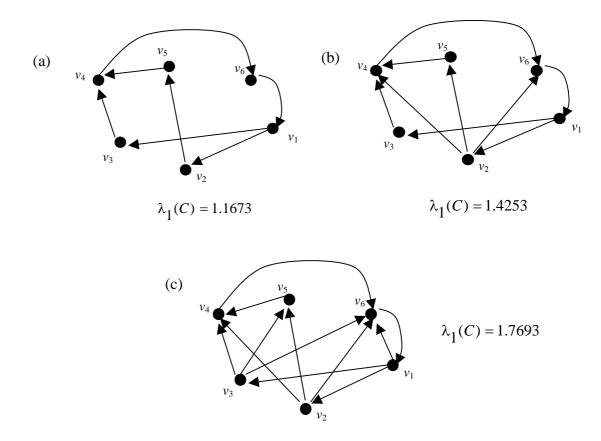
$$\lambda_1(C) = 2.0854$$
 (4.6)

Further, the theorem also states that there exists an eigenvector of *C* corresponding to the value of  $\lambda_1(C)$ , referred to as PF eigenvector (PFE), whose all components are real and non-negative. In this case, the PFE is given as:

$$PFE = \begin{pmatrix} 0.38200\\ 0.18318\\ 0.18318\\ 0.53093\\ 0.35885\\ 0.61344 \end{pmatrix}.$$
(4.7)

Equation 4.7 shows that all the components of the PFE are non-zero. Therefore, the subgraph of the PFE is the entire graph C. Due to the results in Equation 4.6 and Equation 4.7 and by the Proposition 2.4 and Proposition 2.5, it again confirmed to the labeling of graph C as an ACS. This result relates an algebraic property of the graph C, its PFE, to a topological structure, that is its connectedness.

In addition, an interesting connection between Perron-Frobenius eigenvalue  $\lambda_1(C)$  and the irreducible graph is that this value is the measure of multiplicity of internal pathways in the graph. It follows from Perron-Frobenius Theorem for irreducible graphs that  $\lambda_1(C)$  will necessarily increase if any link is added to the graph. Similarly removing any link will decrease  $\lambda_1(C)$ . This can be shown in the following examples in Example 4.2.



Example 4.2:

**Figure 4.3** Changes in the multiplicity of graph indicated by  $\lambda_1(C)$ 

Example 4.2 presented three irreducible subgraphs of *C*. It illustrates that as the number of links increases in the subgraphs, the higher the value of  $\lambda_1(C)$ . Since  $\lambda_1(C)$  measures the multiplicity of the internal pathways of graph *C*, therefore  $\lambda_1(C) = 2.0854$  for the graph *C* signifies the degree of diversity in the interconnection between the variables. The eigenvector corresponding to this eigenvalue  $\lambda_1(C)$  of the graph, known as PFE (Equation 4.7) will be taken to be the attractor for the concentration dynamics in the initial graph (graph *C*) for the model to be developed in the next section.

The discussions on the topological aspect of the graph (namely its connectedness) and its algebraic properties (the structure of the eigenvectors of its adjacency matrix) highlighted in this section provide a good understanding of the graph representing the system. It relates to the concept of ACS, which play an important role in the dynamics of the model studied in this thesis. ACS described the topological make-up of the graph whereas the PFEs described the algebraic nature of the graph. The connection between these two aspects was also discussed and their relationship to the model explaining the clinical waste incineration process will be discussed in the next section.

### 4.3 The Model

Both representations of the clinical waste incineration process in terms of graph and also adjacency matrix signify only on the system's topological structure. The actual dynamical nature of the system can only be represented if this model is coupled with its dynamic variables. Since the concentration of each of the variables in the process changes with time, these values were then considered to be the dynamic variables for the system. This section begins with the discussion on generating and outlining the general framework of the dynamic model (Section 4.3.1). The emphasis of the dynamic model representing the clinical waste

incineration process is on the concentration dynamics and the graph dynamics and both these dynamics will be elaborated in Section 4.3.2.

## 4.3.1 Generating the Framework of the Model

It has been discussed in Section 2.2.2 that the incineration process occurs in both the Primary Combustion Chamber and Secondary Combustion Chamber. In order to materialize the dynamic model, specialization was made with an assumption that the clinical incineration process taken place in <u>one</u> enclosed combustion chamber consisting of primary and secondary combustion chamber containing a set of *s* variables. A given variable *j* can be a catalyst for the production of another variables *i* with some small probability *p*. The presence of *j* in the system causes the concentration of *i* to increase according to the rate equation for catalyzed chemical reactions.

The catalytic relationship is represented using graph, denoted as graph *C* by an arrow from node *j* to node *i* in a directed graph representing the clinical incineration process network. Further specialization made was that the relationship shown by the graph was assumed to occur immediately when the process begins. The graph is completely specified by its adjacency matrix  $C = (c_{ij})$ , *i*, *j* = 1, 2, ... 6.  $c_{ij}$  is unity if there is a link from node *j* to node *i*, that is, if variables *j* catalyzes the production of variable *i*, and zero otherwise. Thus, both the graph and the adjacency matrix play a great role in representing these catalytic interactions between the variables. The adjacency matrix representation of the network is considered in the development of the dynamical model. All these dwell on the structure of the network of the system.

Our concern next is to explore on the possibilities of looking at the dynamics of the process. One thing that we could visualize into was the variables that would change with time. Naturally, it concerns the dynamics of the variables thought to be 'living' on the nodes of the graph. In this case, the dynamics is taken to be the concentrations of each variable, subsequently be noted as the concentration dynamics of the system. The network topology of the system shown by graph C affects the concentration dynamics of these variables in which together they become embodied into one dynamical system. The dynamical system on the network will be modeled as a set of coupled differential equation in which the couplings are specified by the network of interactions.

So far, the discussion mainly focused on the structure of and the behavior of dynamical system on a fixed network. While the study of this static network provides some *insight* into the change of each variable in that particular fixed network, the real nature of the process was not yet prevailed. The network of the clinical waste incineration process is not static. It was also assumed that after a while certain variable would start to deplete or became insignificant in the process. This change would naturally affect the structure of the whole network of the system. This assumption resulted in some modifications to the model of Jain and Krishna, in which the removal of the variable was irreplaceable. The changes of the network signified that the network itself was a dynamic variable.

The above discussions could be explained formally in the following form, symbolizing the general framework of the model for the clinical waste incineration process.

#### 4.3.1.1 The Framework

The clinical incineration process was considered to alter a network, represented by a graph, in discrete steps. The series of graphs produced can be denoted by  $C_n$ , n = 1, 2, ... Each step of the process, taking a graph from  $C_{n-1}$  to  $C_n$ , will be called a 'graph update event'. The following framework defines the changing of the network model consisting of a graph changing, by a series of graph update events along with other system variables and assumptions:

#### **Assumptions**:

- (i) The system was assumed to take place in <u>one</u> combustion chamber comprising both primary and secondary combustion chamber.
- (ii) The network represented by graph C was assumed to denote the interactions of variables at the beginning of the process.
- (iii) After a while, certain variables were assumed to deplete or transform into other form and become insignificant in the process.

**Variables**: The dynamical variables are a directed graph *C* and a variable  $x_i$  associated with each node *i* of the graph. Here, the  $x_i$  represents the concentration of each of the variables. These dynamical variables  $x_i$  can be thought as 'living' on the nodes of the graph.

**Initialization**: To start with, the graph *C* and the variables  $x_i$  are given some initial values. Graph *C* was set to be the initial graph and the relative concentration of each variable at the beginning of the process was taken to be the initial value for  $x_i$ .

### **Dynamics**:

Step 1: First, keeping the graph  $(C_{n-1}$  at step n-1) fixed, the  $x_i$  are evolved for specified time *t* according to a set of differential equations that can be schematically written in the form

$$\dot{x}_i = f_i(C_{n-1}, x_1, x_2, \ldots)$$

where  $f_i$  are certain functions that depend upon the graph  $C_{n-1}$  and on all the  $x_i$  variables.

Step 2: A node may be removed from the graph along with its links. Which node and links are removed from the graph will depend on the  $x_i$  values of the nodes and the graph  $C_{n-1}$ .

Step 3: The node removed is irreplaceable. The remaining nodes will be assigned to a new set of initial values. Repeat all the steps until matrix  $2 \times 2$  was attained.

The framework provides a brief description of the model describing the dynamical system of the clinical incineration process. The three steps prescribed above, described the changes of both the variables and the networks. Step 1 specifies the changes in the variables, which in this case, is the concentration dynamics. On the other hand, Step 2 and Step 3 indicates the changes of the networks denoted as the graph dynamics. These steps produce a new graph, which is the graph at time step  $n, C_n$ . This process, from step 1 onward is iterated until a matrix  $2 \times 2$  is attained.

Adopted and modified from the model illustrated by Jain and Krishna, the three steps procedure describes the clinical waste incineration process. It shows a nonequilibrium statistical mechanics framework of a changing network in the process. The graph is generically in a nonequilibrium state because of the constant removal of the nodes along with their links from the graph. The  $x_i$  variables are also in the nonequilibrium state determined by the function  $f_i$ .

In our model, the species in the incineration process connected in a network are naturally shown by a graph. The above framework was also adopted from Jain and Krishna's model with modifications made particularly to Step 3 in looking at the dynamics of evolution of the network. Since depletion of species occurs during the process of burning, we have foreseen that the removal of nodes should not be replaced and thus resulted in the reducing of the network size. Eventually, this will lead to the species or variables that are present at the end of the process or in other words are the products of the incineration process.

There are two timescales built into this framework. On a timescale much shorter than t, the  $x_i$  variables evolve while the graph remains fixed. On a longer timescale, the graph changes in discrete steps that involve the removal of nodes

along with the links connected to them. The operation of the  $x_i$  dynamics and the graph dynamics on the two timescales illustrates the changes in the incineration process. Over short timescale, the networks in the process are fixed while the concentration change, and over long timescale the network changes because of the depletion or transform into other form or exhaustion of existing variables. Here, the  $x_i$  dynamics and the graph dynamics are interdependent. This feature in shown in the framework as specified below:

- The dependence of the  $x_i$  dynamics on the graph lies in the dependence of the functions  $f_i$  on *C*.
- The dependence of the graph dynamics on x<sub>i</sub> lies in Step 2 and Step 3 in which x<sub>i</sub> to be removed from the network was determined.

A detailed explanation on both the concentration dynamics and the graph dynamics is given in the next section.

# 4.3.2 The Dynamics

The system of a clinical incineration process consists of *s* variables labeled by the index i = 1, 2, ..., s and presented by graph *C*. The  $6 \times 6$  real matrix  $C = (c_{ij})$ , represents the network of the interactions between the variables. The network can be visualized as a directed graph whose nodes represent the variables. In this section, discussions of concentration dynamics and graph dynamics in describing the incineration process are given. It was anticipated that both discussions would provide a good understanding of the dynamic model that would be implemented to the system discussed in next section.

#### **4.3.2.1** Concentration Dynamics

The concentration dynamics equation for a fixed graph  $C = (c_{ij})$  with *s* nodes is given by the set of coupled ordinary differential equations as in Equation 2.1. The dynamics preserves the normalization of **x**, that is  $\sum_{i=1}^{s} \dot{x}_i = 0$ . An important motivation for the choice of the concentration dynamics model for the incineration process is its tractability characteristics. The system as denoted by the equation gives rise to a set of linear change in the  $x_i$  variables.

The model contains another dynamical variable  $\mathbf{x} = (x_1, x_2, ..., x_6)$  where  $x_i$  stands for the relative concentration of the *i*<sup>th</sup> variable. The set of variables  $x_i$  can be thought of as 'living' on the nodes of the graph. The time evolution of  $\mathbf{x}$  depends upon the interaction coefficients *C*, as is usual in the population models. Each variable has a concentration  $y_i$  in the system. Equation 2.3 gives the relative concentration for each of the variables.

The changing of variables experienced in this dynamics stage is expected to reach its stable state at certain time t. This equilibrium state to which all the variables converge can be seen as an **attractor**. An attractor attracts different possible state of the system, so that all trajectories come together at the same point. The key to the changing of the network that will be discussed in the next section is on the **selection** of the variables to be removed from the existing network. Therefore, the variable that has the least concentration in the attractor configuration is the one to be eliminated in a large fluctuation of this hostile environment. The model implements selection by eliminating from the network a variable that has become extinct or has the least contribution to the process. PFE represent the attractor for the concentration dynamics (discussed in section 2.3.4.3).

#### 4.3.2.2 Graph Dynamics

In this section, changing of network of a specific instance of the framework discussed in Section 4.3.1 is presented. The dynamical system described in Section 4.3.2.1 (Equation 2.1) is used in Step 1 of the dynamics, and certain procedures are chosen for Step 2 and 3 to illustrate the changing of the network of the clinical waste incineration process. Both these dynamics can be presented by the following procedures.

#### Result 17

### **Graph Dynamics Procedures**

Step 1: Keeping  $C(s \times s \text{ matrix})$  fixed, x evolved according to Equation 2.1

$$\dot{x}_i = \sum_{j=1}^s c_{ij} x_j - x_i \sum_{j,k=1}^s c_{kj} x_j$$
,

for a time *t*, which is large enough for *x* to get reasonably close to its attractor **X** (Perron Frobenius Eigenvector). We denote  $X_i \equiv x_i(t)$ .

- Step 2: The set *L* of nodes *i* with the least value of  $X_i$  was determined, i.e.  $L = \{ i \in S \mid X_i = \min_{j \in s} X_j, S = \{1, 2, \dots s\} \}$ . This is the set of "least fit" nodes, identifying the relative concentration of a variable in the attractor (or, more specifically, at *t*) with its "fitness" in the environment defined by the graph. One of the least fit nodes is chosen randomly (say  $i_0$ ) and removed from the system along with its links, leaving a graph of s-1 variables.
- Step 3: *C* is now reduced to  $(s-1) \times (s-1)$  matrix. The remaining nodes and links of *C* remain unchanged. All these  $x_i$  ( $0 \le x_i \le 1$ ) are rescaled to keep  $\sum_{i=1}^{s-1} x_i = 1$ . Repeat all the steps until matrix  $2 \times 2$  is attained.

The initial graph for the graph dynamics of the clinical waste incineration process is the graph C (Fig. 3.10c). All the three steps are iterated until  $2 \times 2$  is attained. The graph dynamics of the process is schematically portrayed in Figure 4.4.

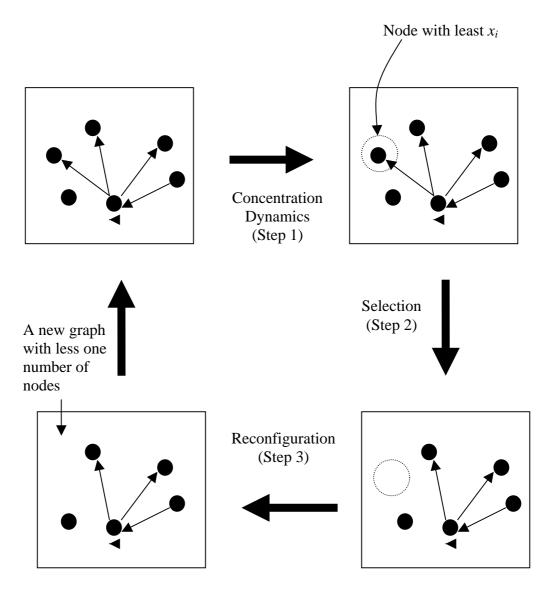


Figure 4.4 Schematic portrayal of the graph dynamics

Figure 4.4 shows that starting with the initial graph, the concentration dynamics is set in motion until the relative concentrations reach their attractor (Step 1). Then one of the nodes with the least relative concentration is removed from the graph (Step 2). The node is removed along with its links and the graph is left with a reduced number of nodes and links (Step 3). This process is then repeated until a graph with at least two nodes is attained.

Step 1 represents the process on its short time scale. On this time scale, the graph remains fixed and each  $x_i$  evolves according to equation 2. Here, all the variables in the system react or evolve according to the links or connectivity among them. This process will proceed until a stable state is achieved, in other words, the process reached its attractor. Here, the attractor is taken as the network's Perron Frobenius eigenvector (PFE) as discussed in Section 3.5.3 and given by Proposition 2.6.

On a longer time scale at discretely sparse intervals (labeled by n = 1, 2,...), the graph itself changes by the elimination of an existing variables from the system. This is represented by step 2. In this case, the variable removed from the system at every update was considered to be completely depleted during the process or it could possibly be due to it was not visibly functioning or its existence was negligent. The end of the evolution of the network was assumed to be when the incineration process completed. The variables left in the network were taken to be the result or the product of the incineration process.

To sum up, it could be seen that the concentration dynamics and the graph dynamics are coupled. The evolution of  $x_i$  depends on the graph C in step 1, and the evolution of C in turn depends on the  $x_i$  through the choice of which node to remove in step 2. The two timescales in the dynamics are basically the short timescale over which the graph is fixed while  $x_i$  evolve and the longer timescale over which the graph is changed. The changing of these networks or the updates of the graphs is further scrutinized in this research and discussed in the following subsection.

#### 4.3.2.3 Graph Updates

The characteristics of the updates of the graphs in Step 2 and Step 3 of the dynamic model were studied. One interesting characteristic about the updates is its relation to sequence.

## **Definition 4.1**

 $n(C_i)$  for i = 0, 1, 2, ..., m is defined as the number of nodes in the  $i^{th}$  updates.

#### Theorem 4.3

The number of nodes in the  $i^{th}$  updates arranged in their consecutive order  $n(C_i)$  for the clinical waste incineration process formed a finite sequence.

# Proof:

The sequence is finite since the value for each term of the sequence connotes to the number of nodes of the graph. Since at each consecutive updates, one node is being removed from the graph, therefore the final term could be determined in the sequence.

This theorem forces us to limit our updating procedure.

It is a decreasing sequence. In fact, it could be proven to be a strictly monotonic decreasing sequence as in the following theorem.

# Theorem 4.4

The number of nodes at the  $k^{th}$  update is given by

$$n(C_k) = n(C_0) - k.$$

## Proof:

Let  $n(C_0)$  be a number of nodes at the initial of the process. Therefore,

 $n(C_1) = n(C_0) - 1$  is the number of nodes at the 1<sup>st</sup> update.  $n(C_2) = n(C_1) - 1 = [n(C_0) - 1] - 1 = n(C_0) - 2$  is the number of nodes at the 2<sup>nd</sup> update  $n(C_3) = n(C_2) - 1 = [n(C_0) - 2] - 1 = n(C_0) - 3$  is the number of nodes at the 3<sup>rd</sup> update : Thus,  $n(C_k) = n(C_{k-1}) - 1 = [n(C_0) - (k-1)] - 1 = n(C_0) - k$  is the number of nodes at the  $k^{th}$  update.

From theorem 4.3, we can get the following corollary.

### **Corollary 4.1**

The number of nodes in the consecutive updates is a strictly monotonic decreasing sequence such that

$$n(C_0) > n(C_1) > n(C_2) > \ldots > n(C_m)$$

### Proof:

By using Theorem 4.2, we have

$$n(C_0), n(C_1) = n(C_0) - 1, n(C_2) = n(C_0) - 2, \dots, n(C_k) = n(C_0) - m.$$

This proved that

$$n(C_0) > n(C_1) > n(C_2) > ... > n(C_m)$$

and the sequence is a strictly monotonic decreasing sequence.

Now, let 
$$S = \{n(C_0), n(C_1), n(C_2), ..., n(C_m)\}$$
 be the set of all the variables

in the process. Since it is a finite sequence and also from Definition 4.1, it could be seen that the maximum of S, denoted as max S is given by

$$\max\{n(C_0), n(C_1), n(C_2), ..., n(C_m)\} = n(C_0).$$

Here, the max is the number of variables at the beginning of the process. In other words, this value can be classified as the input for the process, denoted as

$$S_{\rm in} = n(C_0)$$

The minimum of *S*, denoted by min S is the given by

$$\min\{n(C_0), n(C_1), n(C_2), \dots, n(C_m)\} = n(C_m).$$

The minimum is regarded as the output of the process and can be denoted as:

$$S_{\text{out}} = n(C_m).$$

Here, the initial number of nodes for the graph is the maximum number of nodes. After the destruction process of the incineration, the number of nodes reduces to the least number of nodes at the completion of the process. Next, we will discuss the realization of the three steps in the Graph Dynamic Procedure (Section 4.3.2.2) in describing the clinical waste incineration process.

# 4.4 Implementation

The implementation of the dynamic model to the clinical waste incineration process is discussed in this section. Six main variables are taken to be the key parameters (materials) in the process. These variables are assumed to interact among themselves as soon as the incineration process started. Their interactions and relationships are shown by the graph *C* (Figure 3.10c). We would consider the starting phase here to be the first short timescale of the process (n = 0). We chose the relative concentration of each  $x_i$  at the beginning of the process to be the following values shown in Table 4.1.

i	Name of variable	Weight in kg	Relative concentration of <i>i</i> <sup>th</sup> variable
1	Waste	183.75	0.269
2	Fuel	21	0.031
3	$O_2$	440.35	0.645
4	$CO_2$	0	0
5	СО	0	0
6	Other gaseous + H <sub>2</sub> O	37.5	0.055
	Total	682.6	1.000

**Table 4.1** : The relative concentration of the  $i^{th}$  variable at initial time t = 0

**Note**: Reference was from the material balance flow sheet specified for the clinical waste incineration plant owned by Pantai Medivest Sdn. Bhd.

Table 4.1 gives the following vector **x** referring to the initial value of the relative concentration of the *i*<sup>th</sup> variable at time t = 0.

$$\mathbf{x} = \begin{pmatrix} 0.269\\ 0.031\\ 0.645\\ 0\\ 0\\ 0\\ 0.055 \end{pmatrix}$$
(4.8)

Equation 2.1 together with the given matrix C (Equation 4.2) and vector **x** (Equation 4.8) gives the following results:

$$\begin{pmatrix} \dot{x}_{i} \\ \dot{x}_{2} \\ \dot{x}_{3} \\ \dot{x}_{4} \\ \dot{x}_{5} \\ \dot{x}_{5} \\ \dot{x}_{6} \end{pmatrix} = \begin{pmatrix} -0.453 \\ 0.136 \\ -2.496 \\ 0.945 \\ 0.945 \\ 0.945 \\ 0.709 \end{pmatrix}$$

$$(4.9)$$

On this short timescale, it was anticipated that by keeping the links of the interactions  $(C_0)$  fixed,  $x_i$  evolved according to the rate specified by the Equation 4.9. This evolution of  $x_i$  continued until it reached a particular time whereby a certain variable started to exhaust its value. The variable experiencing this phenomenon corresponds to the least value of the graph's PFE. It was then removed from the system to give way to the remaining variables to concentrate in their interactions. This brought us to the second update of the incineration process.

The graph of the remaining variables, now denoted by  $C_1$  is a different network. Thus, the rate of evolution of the variables would be expected to change or is different from the previous phase. The steps given in the evolution of the network given above was then repeated several times until s = 2. The only different of the later  $C_n$  where n = 1, 2, ... (s-2) from  $C_0$  was that the rate of evolution of  $x_i$  could not be calculated. This was because we cannot get the relative concentration of the variables at the beginning of each phase. This is due the exact time of the transition of each phase could not be specified. Nevertheless, the expected occurrence of the incineration process given by this dynamic model through the three steps evolution of the network can be shown in Table 4.2.

Updates	Variables in graph		olution of	PFE	V <sub>i</sub>
		variables			deleted
$C_0$	$v_1 = Waste$		(-0.45300)	(0.38200)	
	$v_2 = $ Fuel		0.13500	0.18318	
	$v_3 = O_2$	÷ -	-2.49600	0.18318	Fuel
	$v_4 = CO_2$	$\dot{x}_i =$	0.94500	0.53093	
	$v_5 = CO$		0.94500	0.35885	
	$v_6 = H_2 O \& Pollutants$		0.70900	(0.61344)	
$C_1$	$v_1 = Waste$	unspecif	fied	(0.43410)	
	$v_2 = O_2$			0.22521	
	$v_3 = CO_2$			0.51949	$O_2$
	$v_4 = CO$			0.34204	_
	$v_5 = H_2O$ & Pollutant			0.61154	
<i>C</i> <sub>2</sub>	$v_1 = Waste$	unspecified		(0.45033)	
	$v_2 = CO_2$			0.51693	СО
	$v_3 = CO$			0.30727	co
	$v_4 = H_2O \& Pollutant$			0.65998	
<i>C</i> <sub>3</sub>	$v_1 = Waste$	unspecif	fied	(0.54843)	~ ~
	$v_2 = CO_2$			0.41400	$CO_2$
	$v_3 = H_2O$ & Pollutant			0.72652	
$C_4$	$v_1 = Waste$	unspecif	fied	(0.70717)	
	$v_2 = H_2O$ & Pollutant			(0.70717)	

 Table 4.2 : Updates of the incineration process evolution of network

# 4.4.1 Analysis of the Result

Now that we have successfully modeled the dynamic of the clinical waste incineration process through the results summarized in Table 4.2, analysis of the

results have to be acquired in order to see the validity of the model in representing the system. There are two results that we have to *evaluate* corresponding to the two dynamics of the model in accordance with the expectation of the real system. The analyses of these two dynamics are given below.

#### 4.4.1.1 Results of the concentration dynamics

Using the differential equation given by Equation 2.1 to model the concentration dynamics of the process, we expected a linear change in all respected variables at each graph updates. As shown in Table 4.2, only the changes at the initial phase was provided since the relative concentration at the beginning of the consequent networks could not be determined (as explained above). However, the results obtained at this initial phase provide a very good idea and representation of the change of each variable in the system at that particular instance. The change of each variable provided by the model (Equation 4.9 and Table 4.2) is compared to its change based on the real process taken place. Its physical interpretation and analysis of the concentration dynamics of the model at the initial phase is given in the following table (Table 4.3).

xi	Variable	Rate of change	Analysis	
1	Waste	-0.45300	Throughout the incineration process, the waste is being	
			burned. This result in the destruction of the waste into	
			tiny particles and at the same time decreases in sizes into	
			gaseous and tiny particles. The negative rate of change	
			indicates that the amount of waste will decrease.	
2	Fuel	0.13500	Fuel is constantly fed in the secondary chamber in the	
			real process, meaning there is a depletion of its value	
			throughout the process. Thus, the rate of change of Fuel	
			should be negative to indicate the decrease of its value.	
			Even though the value is small, the positive sign for the	
			rate of change of this variable make it inappropriate and	
			incorrect in explaining changes of this variable in the	
			process. Here, the model was not able to represent the	
			real rate of change of fuel in the process.	
3	O <sub>2</sub>	-2.49600	In the incineration process, $O_2$ is being used up to assist	
			the process of burning. The negative rate of change	
			shows that, the amount of $O_2$ decrease in the chamber.	
4	CO <sub>2</sub>	0.94500	These variables are the outputs of the combustion process	
5	CO	0.94500	of the waste. Naturally, the rate is positive showing the	
6	H <sub>2</sub> O &	0.70900	increase of their values throughout the process. In the	
	Other		actual process, the incinerator was monitored so as to	
	Pollutants		produce the minimal amount or emission of CO. The rate	
			of change for CO given here as 0.91700 was still very	
			high and did not actually representing the real process.	

Table 4.3 : Analysis of the concentration dynamics at the initial phase

From the analysis on the changes of the six variables in the initial phase given in Table 4.3, we could see that these results do not actually represent the real process. As such, we could conclude that the concentration dynamics of the consequent graph updates would produce the same outcomes in which the representation of the real system would not be satisfied. Next, let us look at the results on the graph dynamics.

#### 4.4.1.2 Results on the graph dynamics

The graph dynamics or the changes in the network are shown by the deletion of the depleted variable and also by the graph updates as shown by Table 4.2. We can rectify from the table that through the model, fuel will be the first variable to deplete at a given time  $t_1$ . The process then proceeds with only five variables where the next variable to run into exhaustion would be O<sub>2</sub> at time  $t_2$ . The next variable would be CO and then followed by CO<sub>2</sub> at time  $t_3$  and  $t_4$  respectively. Actually, these updates show the depletion sequence of the variables and also the sequence of set of variables remain in the process at any given time t. This is shown below:

- (i) Sequence of depleted variable at a given time *t* :Fuel, O<sub>2</sub>, CO, CO<sub>2</sub>
- (ii) Set of variables remain in the process at a given time t:  $t_0 \rightarrow$  (Waste, Fuel, O<sub>2</sub>, CO<sub>2</sub>, CO, H<sub>2</sub>O & Pollutants)  $t_1 \rightarrow$  (Waste, O<sub>2</sub>, CO<sub>2</sub>, CO, H<sub>2</sub>O & Pollutants)  $t_2 \rightarrow$  (Waste, CO<sub>2</sub>, CO, H<sub>2</sub>O & Pollutants)  $t_3 \rightarrow$  (Waste, CO<sub>2</sub>, H<sub>2</sub>O & Pollutants)  $t_4 \rightarrow$  (Waste, H<sub>2</sub>O & Pollutants)

In looking at the relevancy of the results of these dynamics as compared to the real process, (i) and (ii) provide hints on reviewing the results of the implementation of the model. From (i), we could see that  $O_2$  replenish or being used up so fast in the process. Since we know that oxygen ( $O_2$ ) is vital in any process of burning, this result gives inappropriate and unsatisfactory explanation of the real process. (ii) on the other hand provides us with information of the variables left at the end of the process. In other words, the product of the incineration process could be determined from this graph dynamics of the model. Waste and  $H_2O$  & Other Pollutants are the two variables left at the end of the graph dynamics. By this, we take these two variables being the products of the incineration process. However, according to Bruner (1991), the product of the incineration process is  $CO_2$  and  $H_2O$  & Other Pollutants. Again, this result shown by (ii) of the model does not signify the real clinical waste incineration process. Hence, we deduce that the graph dynamics of the model does not comfortably satisfy the real changes of the network in the process.

### 4.5 Concluding Remarks

This chapter has discussed the framework of the model representing the clinical waste incineration process and the implementation of it to the real system. The changes in variables and the changes in the network of the system have been materialized respectively by the concentration dynamics and graph dynamics of the model. Certain inadequacy and discrepancy of the model in explaining the actual system, as shown in the analysis of both dynamics, is inherent.

### **CHAPTER V**

#### CONCLUSIONS

#### 5.1 Summary

This chapter summarizes the findings presented in the previous chapters and presents the conclusions that can be drawn from them where finally, additional recommendation for future research is suggested.

The modeling of the incineration process has undergone two stages, each of which constitutes separate problems in the study. These problems in turn represent the two objectives of the research work and are separately discussed in two chapters. The first problem, to construct the graphical model that would best explain the dynamic nature of the incineration system, has been discussed in Chapter 3. The graphical model serves as the base for the second problem, discussed in Chapter 4, to construct the model describing the dynamics of the incineration system. The model, adopted and modified from the evolution model proposed by Jain and Krishna, described the two dynamics of the incineration process: the concentration dynamics and the graph dynamics. Autocatalytic set is the key feature of the model.

### 5.2 Significant Findings and Conclusions

The study has successfully modeled the clinical waste incineration process using graph theoretical concept in two different models. All the models illustrate the applications of graph theory in describing the chemical reactions in the incineration process. This study has demonstrated another contribution of the theory which itself is constantly growing in its applications to real world problems and its theoretical aspect.

The first form of the model is symbolized by graphs in which basic graphtheoretic concept was used. Graphical representations both in term of relationship between the input-output variables through and the components of the incinerator and also in term of interactions between variables assumed to play great role in the incineration process have been constructed. Both models are useful in formulating questions about the structure and functioning of the network, which in turn led to the understanding of the incineration process.

The second model incorporated the concept of autocatalysis into graph theory which Jain and Krishna has defined it as Autocatalytic Set (ACS). The model, adopted and modified from the model proposed by Jain and Krishna, employed the autocatalytic set in its construction. The model was able to determine the dynamics of the incineration process namely the concentration dynamics and the graph dynamics. The concentration dynamics of the model was able to ascertain the rate of change of the concentration of each of the variables in the incineration system. The graph dynamics on the other hand was able to describe the change of the network of the process. By this change of the network, the evolution of the species was determined and as a result the product of the incineration process was made known. However, analysis made to the model with respect to the actual process of the incineration system indicates that the model is inadequate in its representation of the incineration process due to the huge assumptions made. Even though the model obtained does not really explain the incineration process, but it does help to narrate the changes of the variables. But further assumptions and approach should be sought for in order to improve the model and the suggestions are made in Section 5.3.

The models exhibit some explanations to the clinical waste incineration process in terms of describing the flow of the system, interaction between variables and also the dynamics of the incineration process. This contributes to the advancement of the mathematical theory in the field. The complexity of the incineration process has made the analysis and predictions in such a system quite difficult, but the graph theoretical concept application in modeling the incineration process as shown by the models was able to overcome the problem. The models describing the dynamics of the process are able to predict the changes of the concentration of the variables and also the changes of the network of the process which otherwise would be difficult.

Modeling the system with new characteristics, such as inserting or deleting variables, would still be easily constructed. The nodes and the links of the graph of the system play great role in the model, so they are the ones that need to be changed in the new model. This signifies the user- friendly feature of the model as compared to the other models developed so far in the incineration process (Section 2.4.2). Any changes to the characteristics of the other models would result in the adjustment made to the differential equations used along with their initial boundaries to accommodate with the insertion or deletion of variables, before the construction of the new model could be made.

#### 5.3 Suggestions for Future Research

The study has shown the capability of graph theory in the modeling of the clinical waste incineration process. It has also revealed and made explicit the thinking processes experienced by us throughout our problem solving activities. Nevertheless there are several avenues could be looked into in future research for the improvement of the model or the extension of this work such as the followings:

a) In this study, attention is given on the chemical species of the incineration process. To provide a better realization of the system, we could explore other parameters to be included in the model such as the temperatures in both chambers of the incineration system (Bruner, 1991). Or we could breakdown  $H_2O$  and pollutants into several components of  $H_2O$  and different type of pollutants so as to look at the individual interactions and changes. In fact, the model could be employed to other system with similar characteristics.

 b) Equation 2.1 used in representing the concentration dynamics of the incineration process could be replaced with other equations. Such equations could be of the following replicator equation (Hofbauer and Sigmund, 1988):

$$\dot{x}_i = x_i \left[ \sum_{j=1}^s c_{ij} x_j - \sum_{k,j=1}^s x_k c_{kj} x_j \right].$$

The name 'replicator' comes from the fact that the equation models selfreplicating species, for example in model ecosystems (Hofbauer and Sigmund, 1988).

c) Since the inception of Fuzzy graph theory (Zadeh, 1965), the theory of fuzzy sets has evolved in many directions, and finds its applications in many branches of engineering and technology (Klir & Yuan, 1997). With this, fuzzy graph could be opted in this research as an alternative approach to model the clinical waste incineration process. In fact, the strictly given value of 0 and 1 given to the link strengths of the network described in Chapter 4 could have contributed to such results that inadequately explained the process. Considering the real process of the system, the variability of the link strengths must be adhered. Therefore,  $c_{ij}$ , when non-zero, are allowed to take any value in the interval of (0,1]. The dynamic model of the clinical waste incineration process based on fuzzy graph theoretical concept could then be proposed.

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# APPENDIX A

The original Schematic Diagram and the Material Balance of the Clinical Waste Incineration Plant in Malacca

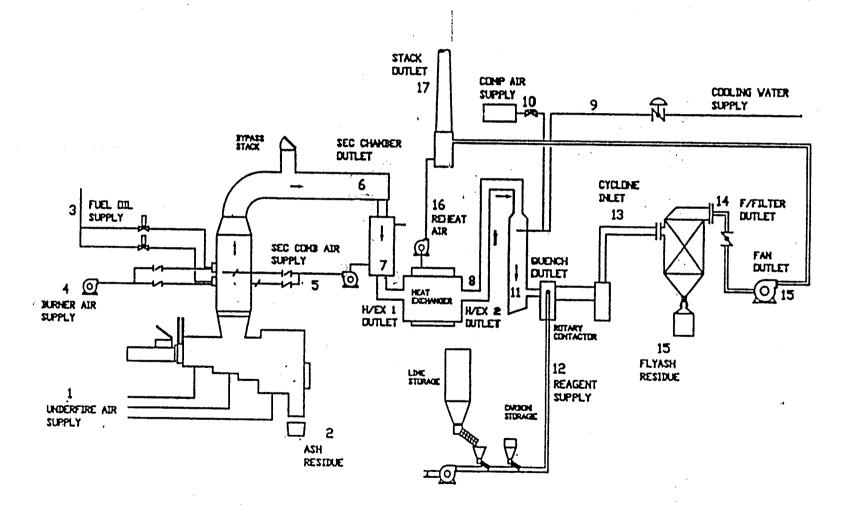


Figure A.1: The Original Schematic Diagram of the Clinical Waste Incineration Plant in Malacca

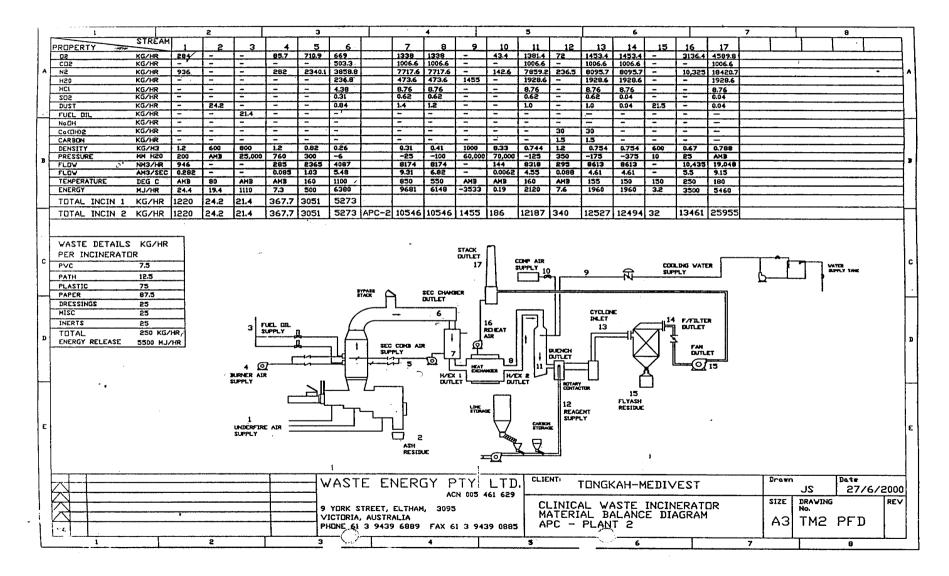


Figure A.2: Material Balance Chart for the Clinical Waste Incineration Plant in Malacca

**APPENDIX B** 

Samples of Data Collected at the Clinical Waste Incineration Plant in Malacca

Table B1: Sample of Data Collected at the Clinical Waste Incineration Plant in Malacca – Dated 21 November 1999

Y TONGKAH MEDIMEST SIDN BHD INCINERATOR PLANT BILIKIT RAMBAI 

Environmental Management System

Co No 224192-H.

Quality Management System Commercial in Confidence

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Table B2: Sample of Data Collected at the Clinical Waste Incineration Plant in Malacca – Dated 22 November 1999

TONGKAH MEDIVEST SDN BHD INCINERATOR PLANT BUKIT RAMBAI

Environmental Management System Quality Management System Commercial in Confidence

#### INCINERATION DAILY LOG

DATE: 22 / 11/99

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Table B3: Sample of Data Collected at the Clinical Waste Incineration Plant in Malacca – Dated 23 November 1999

TONGKAH MEDIVEST SON BHD INCINERATOR PLANT BUKT RAMBAI

Environmental Management System Quality Management System Commercial in Confidence

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#### INCINERATION DAILY LOG

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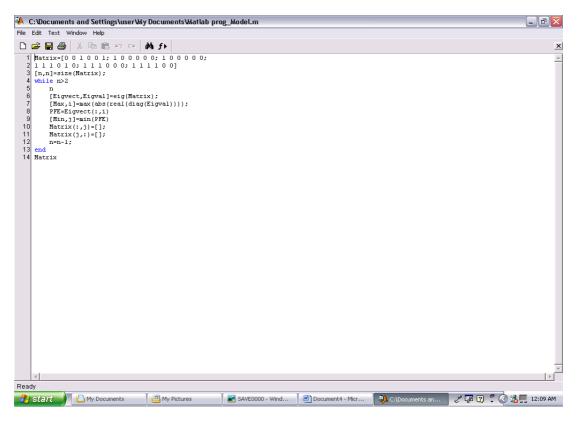
POF/FRW/160 Version 1.00 1<sup>st</sup> July 1999

# **APPENDIX C**

Programs Used in Determining the Changes of Network in the Models

Programs Used in Determining the Changes of Network in Models

## C.1 Model Using ACS



# C.2 Model Using FACS

