



**KTH Industrial Engineering  
and Management**

# **Numerical Study on Combustion Features of Gasified Biomass Gas**

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## Abstract

There is a great interest to develop biomass combustion systems for industrial and utility applications. Improved biomass energy conversion systems are designed to provide better combustion efficiencies and environmental friendly conditions, as well as the fuel flexibility options in various applications. The gas derived from the gasification process of biomass is considered as one of the potential candidates to substitute traditional fuels in a combustion process. However, the gas composition from the gasification process may have a wide range of variation depending on the methods and fuel sources. The better understanding of the combustion features for the Gasified Biomass Gas (GBG) is essential for the development of combustion devices to be operated efficiently and safely at the user-end.

The objective of the current study is therefore aiming to achieve data associated with the combustion features of GBG fuel for improving the efficiency and stability of combustion process. The numerical result is achieved from the kinetic models of premixed combustion with a wide range of operating ranges and variety of gas compositions. The numerical result is compared with experimental data to provide a better understanding of the combustion process for GBG fuel.

In this thesis the laminar flame speed and ignition delay time of the GBG fuel are analyzed, using 1-D premixed flame model and constant-volume model respectively. The result from different kinetics are evaluated and compared with experimental data. The influences of initial temperature, pressure and equivalence ratio are considered, as well as the variation of gas compositions. While the general agreement is reached between the numerical result and experimental data for laminar flame speed prediction, deviations are discovered at fuel-rich region and increased initial temperature. For the ignition delay time, deviations are found in the low-temperature and low pressure regime. The empirical equations considering the influence of initial temperature, pressure and equivalence ratio are developed for laminar flame speed and ignition delay times. The influence of major compositions such as CO, H<sub>2</sub> and hydrocarbons are discussed in details in the thesis. Furthermore, a simplified kinetic model is developed and optimized based on the evaluation of existing kinetics for GBG fuel combustion. The simplified kinetic model is expected to be used for simulating the complex combustion process of GBG fuel in future studies.

**Keywords:** Kinetic model; gasified biomass gas; premixed combustion; laminar flame speed; ignition delay time



## Sammanfattning

Det finns ett stort intresse för att utveckla energisystem baserade på förbränning av biomassa för industriella och allmännyttiga applikationer. Förbättrade system för omvandling av biomassa utformas för att ge bättre förbränningsverkningsgrad och miljövänliga förhållanden, liksom för att ge bränsleflexibilitet i olika applikationer. Gasen härrörande från förgasningsprocessen av biomassa anses som en av de potentiella kandidaterna att ersätta traditionella bränslen i en förbränningsprocess. Emellertid kan kompositionen av gasen från förgasningsprocessen variera mycket beroende på valda metoder och bränslekällor. En bättre förståelse av förbränningsfunktioner för gas från förgasad biomassa (GBG) är avgörande för utvecklingen av förbränningssystem som ska drivas effektivt och säkert hos slutanvändaren.

Syftet med den aktuella studien är att samla och analysera data som är associerade med förbränning av GBG bränsle för att förbättra effektiviteten i förbränningsprocessen. Numeriska resultat erhålls från kinetiska modeller av förblandad förbränning för ett brett driftsområde och olika gassammansättningar. Det numeriska resultatet jämförs med experimentella data för att ge en bättre förståelse av förbränningsprocessen för GBG bränsle.

I denna avhandling har laminära flamhastigheten och tändfördröjningstiden för GBG bränsle analyserats, med användning av en 1-D förblandad flam-modell respektive en konstant-volymmodell. Resultatet från olika sorters kinetik utvärderas och jämförs med experimentella data. Inflytandet av begynnelsestemperatur, tryck och ekvivalenskvot betraktas, liksom gasens sammansättning. Medan generell överensstämmelse nås mellan det numeriska resultatet och experimentella data för att förutsäga den laminära flamhastigheten har avvikelser upptäckts vid driftförhållanden med feta bränsleblandningar och förhöjd begynnelsestemperatur. För tändfördröjningen har avvikelser identifierats i driftområden med låg temperatur och lågt tryck. De empiriska ekvationerna som avser begynnelsestemperatur, tryck och ekvivalenskvot har utvecklats för laminära flamhastighet och tändfördröjningstider. Inverkan av domierande bränslekomponenter såsom CO, H<sub>2</sub> och kolväten diskuteras i detalj i avhandlingen. Vidare har en förenklad kinetisk modell utvecklats och optimerats baserat på utvärderingen av existerande kinetik för förbränning av GBG bränsle. Den förenklade kinetiska modellen förväntas användas för att simulera den komplexa förbränningsprocessen för GBG bränsle i framtida studier.

**Nyckelord:** Kinetisk modell; förgasad biomassa; förblandad förbränning; laminär flamhastighet; tändfördröjningstid



# Preface

The licentiate thesis is supported by the division of Heat and Power Technology (HPT), School of Industrial Engineering and Management and the Chinese Scholarship Council (CSC). The current study which is presented in this thesis has been considered as a part of the PhD project for understanding the combustion process of alternative fuels in gas turbine combustor. The research result in current work is based on 3 papers. The papers are appended at the end of the thesis.

- I Zhang, Xiaoxiang, Nur Farizan Munjat, Jeevan Jayasuriya, Reza Fakhrai, and Torsten Fransson. "Evaluation of Reduced Kinetics in Simulation of Gasified Biomass Gas Combustion." *ASME Turbo Expo 2013: Turbine Technical Conference and Exposition*. American Society of Mechanical Engineers, 2013.
- II Zhang, Xiaoxiang, Jeevan Jayasuriya, and Torsten Fransson. "Kinetic Evaluation of the Laminar Flame Speed for Biomass Derived Gas Combustion." *Submitted to the Elsevier journal, Biomass and Bioenergy*. Paper is currently under review..
- III Zhang, Xiaoxiang, Jeevan Jayasuriya, and Torsten Fransson. "Kinetic Study on Ignition Delay Time of Biomass Derived Gas Combustion." *Submitted to the Elsevier journal, Applied Energy*. Paper is currently under review..





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# Nomenclature and Abbreviations

## Symbols

---

|               |                                 |                  |
|---------------|---------------------------------|------------------|
| $A$           | Pre-exponential factor          | $mol, cm, s, K$  |
| $A_b$         | Area of flame reaction zone     | $m^2$            |
| $c_p$         | Constant-pressure specific heat | $J/kg \cdot K$   |
| $\bar{c}_v$   | Constant-volume specific heat   | $J/kmol \cdot K$ |
| $D_i$         | Mass diffusivity                | $m^2/s$          |
| $\mathcal{D}$ | Binary diffusion coefficient    | $m^2/s$          |
| $E_A$         | Activation Energy               | $cal/mol$        |
| $h$           | Enthalpy                        | $cal/mol$        |
| $J$           | Jacobian matrix                 | –                |
| $k$           | Reaction rate coefficient       | –                |
| $Le$          | Lewis Number                    | –                |
| $m$           | Mass                            | $kg$             |
| $\dot{m}$     | Mass flux                       | $kg/s \cdot m^2$ |
| $P$           | Pressure                        | $atm$            |
| $P_u$         | Pressure of unburnt gas mixture | $atm$            |

|              |                                      |                  |
|--------------|--------------------------------------|------------------|
| $\dot{Q}$    | Heat flux                            | $W/m^2$          |
| $R_u$        | Universal gas constant               | $J/kmol \cdot K$ |
| $S_L$        | Laminar flame speed                  | $m/s$            |
| $t$          | Time                                 | $s$              |
| $T$          | Temperature                          | $K$              |
| $T_u$        | Temperature of unburnt gas mixture   | $K$              |
| $T_i$        | Initial temperature                  | $K$              |
| $u, \bar{u}$ | Internal energy                      | $J/kmol, J/kg$   |
| $v$          | Average velocity                     | $m/s$            |
| $V$          | Volume                               | $m^3$            |
| $x$          | Distance                             | $m$              |
| $X$          | Mole fraction                        | –                |
| $Y$          | Mass fraction                        | –                |
| $Y_u$        | Mass fraction of unburnt gas mixture | –                |
| $\alpha$     | Coefficient                          | –                |
| $\beta$      | Empirical parameter                  | –                |
| $\Delta H$   | Specific enthalpy                    | $J/kg$           |
| $\theta$     | Coefficient                          | –                |
| $\lambda$    | Thermal conductivity                 | $W/m \cdot K$    |
| $\dot{\mu}$  | Volumetric flow rate                 | $m^3/s$          |
| $\rho$       | Density                              | $kg/m^3$         |
| $\tau_{ign}$ | Ignition delay time                  | $\mu s$          |
| $\phi$       | Equivalence ratio                    | –                |
| $\Phi$       | Solution vector                      | –                |

|                |                   |                    |
|----------------|-------------------|--------------------|
| $\psi$         | Relaxation factor | –                  |
| $\dot{\omega}$ | Production rate   | $kmol/s \cdot m^3$ |

---

## Abbreviations

---

|      |                                     |   |
|------|-------------------------------------|---|
| CFD  | Computational Fluid Dynamics        | – |
| CSP  | Computational Singular Perturbation | – |
| GBG  | Gasified Biomass Gas                | – |
| ILDm | Intrinsic low-dimensional manifolds | – |
| LHV  | Lower Heating Value                 | – |
| MFC  | Mass Flow Controller                | – |
| ODEs | Ordinary Differential Equations     | – |
| PSR  | Perfect Stirred Reactor             | – |

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# Chapter 1

## Introduction

### 1.1 Context and Motivation

Combustion has been used for keeping us warm, cooking food, giving light and generating energy for hundred thousands of years, and is constantly doing so today. A quick glance around our everyday life shows the importance of combustion, from the food we cook to the car we drive, from the heating system in the building to the propulsion system in the rocket. With the increase of new energy sources such as nuclear energy, hydro-power, wind and solar energy, the combustion, as the most traditional method of producing energy still provides us with more than 90 percent of total energy consumption today. The percentage is even higher in the large developing country like India or China.

Despite of the importance of combustion in human society today, traditional fuels such as fossil fuels were considered as cheap and abundant are proved to be not sustainable. With the decrease quantities and increase price of fossil fuels, new alternative fuel sources are urgently needed. Another disadvantage associated with traditional combustion process is the emissions which related to environmental problems. Primary pollution considered to be related to smog, acid rains, ozone depletion and various health problems. Carbon dioxide which was also considered as clean products of the combustion process is now accused as the main responsible for greenhouse effect which causes the global climate change. A report from the International

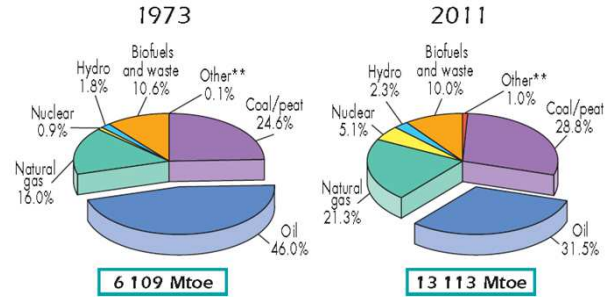


Figure 1.1: 1973 and 2011 fuel shares of Total Primary Energy Supply. (IEA, 2013)

Panel on Climate Change (IPCC) has shown a high possibility of a relationship between the greenhouse gas emission and human activities, the most essential one is considered to be the insufficient combustion process (IEA, 2013).

The combustor as a part of gas turbine is set between the compressor and the turbine. A general type of gas turbine combustion is shown in Figure 1.2. Generally, the function of gas turbine combustor is to mix the fuel and high pressure air from the compressor together and provide a well combustion process with the mixture to achieve the effective release of chemical energy from the fuel. The energy is released which will be transferred to the thermal energy of high temperature gas to improve the potential capacity before the turbine.

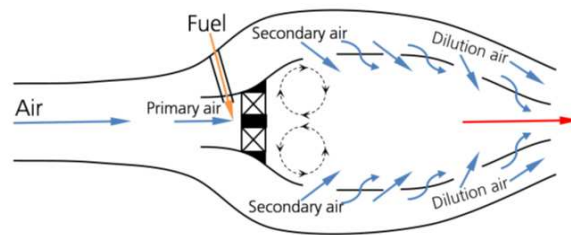


Figure 1.2: Schematic illustration of a general combustor (Sigfrid, 2013).

The gas turbine community has been showing more and more interests in alternative fuels, which may cope with the constant increase of fossil fuel price and higher standards of emission regulation (Lefebvre, 1998). Gasi-fied Biomass Gas (GBG) is considered as carbon dioxide neutral and its constituents are dominated by methane, which could be directly upgraded to replace natural gas as a fuel for gas turbine combustor (Munajat *et al.*, 2012). However, there is a lack of knowledge about the combustion of GBG gas, and problems such as distinguish and flashback of the flame are foreseen to occur when directly burning it with traditional combustors designed and optimized for fossil fuels. The problems of how should it be burnt become more important than ever, especially when it comes to the design of the combustion process for unproven new fuels.

## 1.2 Basic Features of GBG Fuel

The gas compositions generated from the gasification process of biomass is known as gasified biomass gas (GBG) fuel. It has multiple advantages such as widely distributed, relatively high amounts and low in costs when compared with traditional fuels and other alternative energy sources. The process of biomass utilization is considered to be carbon neutralized when the environmental emission is put into concern. On the other hand, the GBG fuel has its own features which is required to be studied before it could be used in gas turbine combustors. Several basic features of the GBG fuel are listed as follows:

- GBG fuel has relatively lower calorific value compared to natural gas. Due to the various processes and biomass resources, the low heating value of a typical gas composition derived directly from the gasification process of biomass ranges from 3.7 to 8.4  $ME/Nm^3$  (when air is used as gasification agent). And the low heating value for natural gas is around 36.5  $MJ/m^3$ , which is 5-10 times higher than GBG fuels. Therefore the time for complete combustion will be longer and the flow rate need to be increased to meet the requirement of combustion efficiency (Terry Ford, 1990). In addition, there are additional components in the GBG fuel such as CO and H<sub>2</sub>, together with the water vapour and tars. These conditions may limit the operation range of the gas turbine, and cause a change in flame stability, temperature

distribution and flame propagation. For instance, the higher level of hydrogen may cause the flashback of flame due to the smaller molecule and faster reaction rate it has.

- The fuel composition can vary greatly when operating the GBG fuels instead of traditional fossil fuels. The variations are mainly caused by the variation in biomass resources and gasification procedures. Although most GBG fuels contain hydrogen and carbon monoxide as main compositions (Ouimette and Seers, 2009; Liu *et al.*, 2010; Vu *et al.*, 2011), potential variables such as the carbon dioxide, hydrocarbon species, water and nitrogen can have a pronounced effect on combustion processes (Chaos and Dryer, 2008) as well as the varying ratios of hydrogen/carbon monoxide.
- Another concern is the substantial NO<sub>x</sub> emissions, which may be caused by the combustion of GBG fuel. As the traditional combustor has been designed for natural gas with a lean, premixed combustion to minimize the pollutant emissions, the similar approach for GBG fuels has shown a requirement of further studying on the fluid dynamics and chemical kinetic models. Figure 1.3 shows the estimation results of NO<sub>x</sub> concentration for syngas combustion, which has a similar composition as GBG fuels. The numerical results of NO<sub>x</sub> emission is shown considering the influence of residence time and pressure with the stoichiometric condition.

### 1.3 Numerical Study on Combustion Features

Numerical method is one of the most important approaches to study the combustion process. To compare with the experimental study which requires considerable cost of time and resources, the numerical method of combustion study could provide us more detailed data with relatively lower costs if the appropriate theory and model is adopted. The detailed data which is achieved from numerical study could also be used for the further understanding of the fundamental of the combustion process. Moreover, there is always a requirement to understand the fundamental of new fuels – especially when their components are flexible – before the prototype testing facility can be built. The flexibility of combustor burning different kinds of fuel gases with minimized change is important in modern industrial appli-

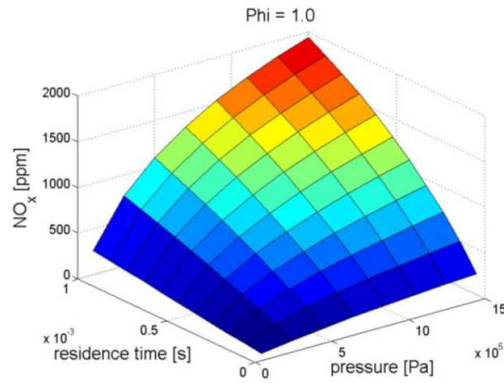


Figure 1.3: NO<sub>x</sub> concentration estimated by a single PSR for Syngas(Sigfrid *et al.*, 2013).

cations. With the fast development of computational resources in the last few decades, a lot of attention has been attracted to develop the numerical methods for combustion researches.

Despite the advantage of the numerical study of the combustion process, there are still challenges in developing the suitable approaches to accurately predict the combustion performance (Veynante *et al.*, 1994; Poinso *et al.*, 2005). One of the important problems is to reproduce the basic features of combustion processes with appropriate chemical kinetics. The chemical kinetic needs to be put into concern when considering the features of ignition, extinction, flame stability and flame propagation. At the mean while, although a detailed kinetic has been always preferable as it can provide more accurate and detailed data of the chemical process, it could also lead to the difficulty of numerical calculation with stiff equations. Therefore an appropriate selected and optimized kinetic is required for specific fuels.

To overcome these issues associated with the utilization of GBG fuels, a improved understanding of the combustion process is essential from the respective of both physical and chemical reactions. The basic features of a specific kind of fuels which describes the fundamental combustion phenomenon can have an combined influence in complex combustion process such as in the industrial gas turbine combustors. For instance, the propaga-

tion of a turbulent combustion have an essential association with the laminar flame speed and thickness. Moreover, the basic combustion features which is achieved from precisely controlled experiments with irrelevant influences excluded are considered to be more accurate. The numerical models which are used to reproduce these basic phenomenon are also considered to be more reliable to use. Therefore, the basic features of the combustion process should be studied in details before the complex combustion phenomenon is put into concern.

There are several comprehensive chemical kinetics which have been developed for natural gas and hydrocarbon combustions with thoroughly validated with experiments carried out with a range of operating conditions. With the CO/H<sub>2</sub>/O<sub>2</sub> system has also been studied in detail and thought to be reasonably well established and understood (Gardiner Jr and Olson, 1980; Westbrook and Dryer, 1984; Chaos and Dryer, 2008), there are requirements to test and updated comprehensive kinetic models for the oxidation of H<sub>2</sub>/CO mixtures (Sun *et al.*, 2007; Chaos and Dryer, 2010; Yan *et al.*, 2011).

Furthermore, few simplified kinetics which can be used to achieve reasonable prediction for specific GBG fuel have been developed in former studies (Nikolaou *et al.*, 2012; Abou-Taouk *et al.*, 2013; Boivin *et al.*, 2013). The original simplified kinetics which were developed for natural gas combustion (Charles and Dryer, 1981; Westbrook and Dryer, 1984; Jones and Lindstedt, 1988; Zsély *et al.*, 2009) need to be validated and optimized before implementing with CFD simulation of GBG fuel combustion.

## 1.4 Objective of the Work

The main objective of current work is to study the basic features of GBG fuel combustion for the purpose of improving the combustion performance of GBG fuel. The combustion process which is put into concern in current study is the premixed type of flame since it has a wide utilization in gas turbine combustor. Besides the experimental approach of gas turbine combustor design, which can be quite limited by the access to the considered devices and high cost with manufacturing and operation, a numerical approach to combustion problem is adopted as major method in current study. The basic features of the GBG fuel combustion is evaluated with the comparison of various numerical results, as well as the comparison of the



experimental data.

The detailed objectives of current study are listed as follows:

- As the turbulent flame propagation is essentially influenced by the laminar flame speed of fuels, the laminar flame speed of a typical GBG fuel is studied with both experimental data and the results from numerical calculation of chemical kinetics. The variations of the fuel compositions and equivalence ratio is considered, as well as the variation of initial temperature and pressure.
- Despite the influence of laminar flame speed, the combustion process is also highly influenced by the ignition delay time of the fuel. The autoignition delay time of typical GBG fuels and Syngas is studied with a review of published data and numerical kinetic models. The influences of the fuel compositions and equivalence ratio are evaluated, as well as the initial temperature and pressure. The empirical equations are proposed and their reliability is also discussed.
- To validate the existing kinetics for GBG fuel combustion with the experimental data. The simplified kinetic is optimized and validated for GBG fuel combustion to be implemented with further CFD simulations. The validation and optimization is done based on the laminar flame speed.

## 1.5 Methodology

The methodology which used in the current study has already been briefly mentioned in previous sections. One of the essential parameters which put into concern here is the laminar flame speed, which has close relation to the turbulent flame speed and the flame stability. It also takes important roles in the phenomenon of flashback and blowoff. Another focused feature in the current study is the ignition delay time, which has an important consequence on the reactive system and directly controls the combustion dynamics inside the combustor. Since the compositions of the GBG fuels vary depending on the source of biomass and processing methods, the main focus in current study is given on the kinetic evaluation of  $H_2 - CO$  system as  $H_2/CO$  is the dominating combustible components of the GBG fuel mixture

The numerical models combined with the developed chemical kinetics are adopted as the main tool to study the basic features of GBG fuel combustion, as well as the supplement from experimental data. The basic features which studied in the current study are relatively stable and symmetrically distributed compared with the combustion features in a complex industrial combustion. Therefore, the numerical calculation based on the 1-D model is carried out in the study.

The method which uses the theoretical models of reaction kinetics to calculate the basic features of specific combustion process has already been developed rapidly since early 20th century. And it is considered to be fairly accurate to predict the basic combustion features when using with specific combustion fuels such as hydrogen or methane. However, due to the complexity of combustion processes, there is always a challenge to correctly predict the flame phenomenon with a wide range of operating conditions, especially with high ambient temperature and high pressure. The addition of reaction dynamics in the mass and energy conservation equations can also cause the instability of closure models and therefore influence the robustness of the numerical system. Moreover, the extra effort is always required to use the developed chemical kinetics for new fuels. The evaluation is done in the current study to validate the utilization of existing kinetics for GBG fuels.

## 1.6 Outline of Thesis

- Chapter 2 is a state of art for the chemical kinetic study for gas combustion. The main context covers the development of detailed kinetics, the requirement to develop the reduced and simplified global kinetics for different fuels, as well as their applications combined with different scales of the combustion processes. A review concerning the computational power for various scales of kinetic sets is also covered in this chapter.
- Chapter 3 is an introduction to the numerical models which are used to calculate the laminar flame speed and ignition delay time with chemical kinetics. 1-D adiabatic laminar flame speed is used to predict the laminar flame speed of GBG fuels, while the constant volume and adiabatic reactor is used to predict the ignition delay time.

- Chapter 4 is the description of the work of kinetic evaluation of Gasified Biomass Gas combustion features. The optimization of Gasified Biomass Gas combustion through the validation of experimental data and detailed combustion kinetic simulations is also presented in the chapter. The results associated with paper 1, 2 and 3 are presented in this chapter.
- Chapter 5 is the general conclusion of current work.



## Chapter 2

# Chemical Kinetics for Combustion – State of Art

The chemical kinetics of the combustion plays an essential role in understanding of the combustion process (Westbrook *et al.*, 2009). The objective of studying chemical kinetics usually relates to the calculation of combustion rates, which is constantly evolving with the time and flow conditions (Lefebvre, 1998). The chemical reaction rate controls the generation and destruction of pollutants, therefore, is usually put into concern when emission problems may occur in the combustion process (Li *et al.*, 1999). On the other hand, the ignition and extinction of flames also have a theoretical fundamental in chemistry reactions, which should be treated with appropriate chemical kinetics in combustion simulations (Jones and Lindstedt, 1988; Frassoldati *et al.*, 2009, 2007). Progresses have been made in past decades through both experimental and theoretical studies of combustion processes.

### 2.1 Chemical Process of Combustion

There are two ways to study the chemical processes of combustion in general. The classical methods are based on the analysis of original experimental data, then establish the reaction parameters through the analysis. This method highly relies on the ability of detection and analyse the intermediates during the reaction process (Westbrook *et al.*, 2005). Another routine is to go through the whole chemical process from the microscale point of

view, normally based on the collision between the reactant molecules. Fig. 2.1 shows a study with  $\text{CH}_3$  roaming kinetic which was done recently (Heazlewood *et al.*, 2008). The numerical study based on quantum chemistry is usually required to calculate the potential energy surface for the reaction system and the quantum mechanic study is also needed to set up the motion trails. Although the method based on the quantum theory is believed to be more fundamental, this is still difficult to get the complete potential energy surface except for very few simple reactions. The reaction kinetics study today is therefore mostly based on the first method with the classical statistical analysis (Westbrook *et al.*, 2005), and this is the only method which is put into concern in current study.

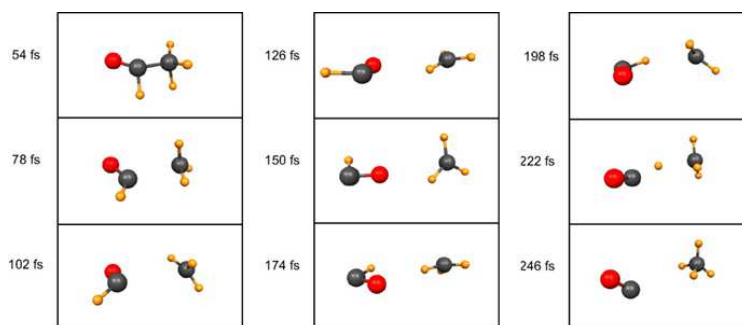


Figure 2.1: A sample  $\text{CH}_3$  roaming trajectory leading to  $\text{CH}_4 + \text{CO}$  via a roaming pathway.

The study of chemical kinetics of combustion process started almost same as the modern chemistry was established. With basic characteristics of gases and balanced equations established the fundamental of chemical analysis, the kinetic study has developed rapidly since the early 20th century (Turns Stephen, 2000). In the first half of the 20th century, most efforts have been put on to find out the empirical equations for chemical process, and to define the parameters related to it (Westbrook *et al.*, 2005). The research on elementary reactions started in the late 20th century with the development of free radical chain reactions (Dryer and Glassman, 1973). There is also a requirement for better detection of activity intermediates with the development of new measurement technologies. The ability for detecting the temporary radicals has reached 10-10s and more and more reaction routes have been added to the kinetic system (Westbrook *et al.*, 2005). However,

due to the equilibrium assumption which is usually needed to establish the chemical kinetics, most kinetics are limited to a certain range of operating conditions, with relatively limited information about real reactions and need to be treated carefully for the fast reactions which happened in combustion processes. The detailed kinetic developments with the experimental findings will be discussed in the following chapters, as well as performance and limitations.

At the same time, although a tremendous amount of progress has been made, the problem of predicting the detailed process of combustion in a complex flow field, where both fluid mechanics and chemistry are treated from the first principles, has not yet been fully solved (Westbrook *et al.*, 2005). The computational resource which is required for the CFD solution of a combustion process is usually huge and makes the implement of detailed chemical kinetics to be hard as these kinetics usually contains thousands of reactions to simulate and hard to get it converged (Frassoldati *et al.*, 2009). There is a demand for appropriate developed reduced or simplified kinetics which could be used with CFD model and provide certain levels of information with adequate accuracy. The development of simplified kinetics will also be discussed in the following chapters.

## 2.2 Detailed Kinetics Research for Gasified Biomass

The elementary reactions which used in the chemical kinetics represent a specific reaction rate. The reactants collide with sufficient activation energy to change the structure and form new products. A typical bimolecular reaction in which  $\dot{A}$  and  $\dot{B}$  as reactants and  $\dot{C}$  and  $\dot{D}$  as products can be written as equation 2.1:



The rate of the reaction is proportional to the combined product of the concentrations of the reactants with a power equal to their stoichiometric coefficient respectively according to the experimental study. In most chemical reactions which have been developed, the reaction rates are usually determined by the empirical Arrhenius form as below (Glassman and Yetter, 2008),

$$k(T) = AT^\beta \exp(-E_A/R_u T) \quad (2.2)$$

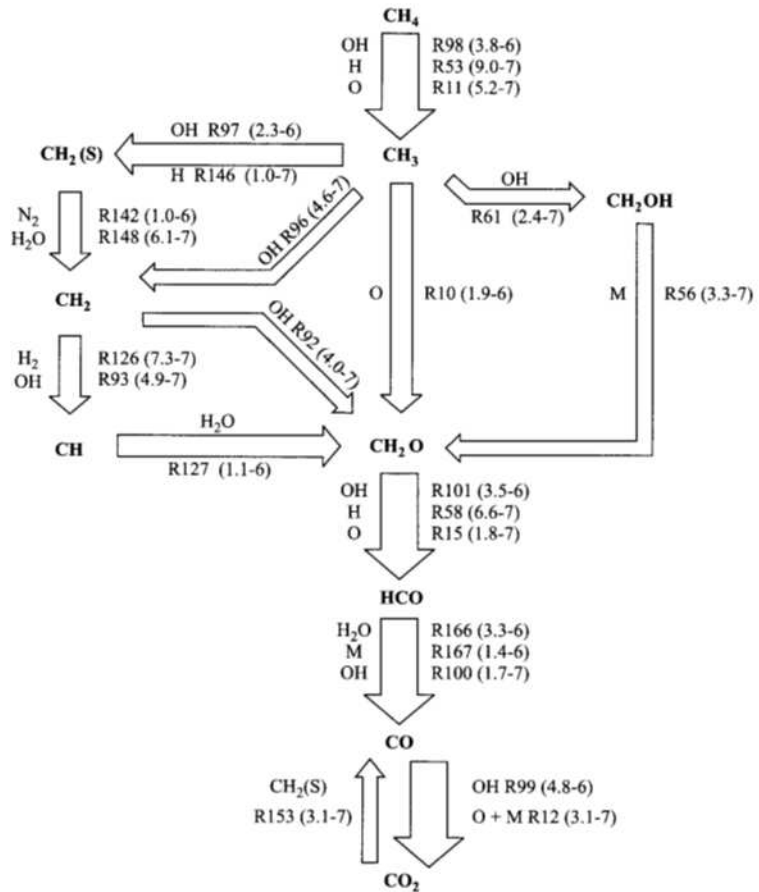


Figure 2.2: High-temperature reaction pathway diagram for combustion methane in a well-stirred reactor at  $T=2200$  K and  $P=1$  atm for a 0.1 s residence time (Turns Stephen, 2000)



Where  $A$  is the pre-exponential factor which has the same unit as  $k(T)$ ;  $E_A$  is the activation energy that required for the reaction to take place and  $b$  is the empirical parameter which related to the temperature change. The attempting of using chemical kinetics for numerical solution was attempted since 1950s by Curtiss and Hirschfelder (Curtiss and Hirschfelder, 1952). But there were difficulties to solve the kinetic equations for real flames before 1975, which the development for solving the stiff equation were available (Westbrook *et al.*, 2005). At the mean while, due to the transient feature of combustion process, the chemical time scales is put into concern in certain cases, especially when it is comparable to other time scales. The chemical time scales is defined as the time required for the concentration of reactants to decrease from initial value to a value equal to  $1/e$  times of the initial value:

$$\tau_c = \frac{\ln(e + (1 - e))([\dot{A}]_0/[\dot{B}]_0)}{([\dot{B}]_0 - [\dot{A}]_0)k(T)} \quad (2.3)$$

where  $[ ]$  refer to the concentration of specific species.

F.L. Dryer and I. Glassman (Dryer and Glassman, 1973) studied the high-temperature oxidation of CO and CH<sub>4</sub> in 1970s using the turbulent-flow reactor. The importance of hydroxyl radical concentration and oxygen-atom attack on methane were mentioned in their work for the CO oxidation and methane/oxygen reactions respectively. Their results also suggested that the hydrogen attack on methyl radicals was important for methane disappearance and should be evaluated under high temperature conditions. The over-all rate expressions for CO and CH<sub>4</sub> oxidation were achieved from the experimental data (Dryer and Glassman, 1973). However, the methane oxidation mechanism was considered to be simple, consisting only methyl radicals and formaldehyde. Later, at the beginning of 1980s, Charles Westbrook and Frederick Dryer reviewed and developed the chemical kinetic model for the general hydrocarbon combustion under high temperature conditions (Westbrook and Dryer, 1984). Their work of kinetic modification was carried out together with the sensitivity analysis. Specific mechanisms which had important affects to the combustion process such as hydrogen oxidation, ozone decomposition and the yield of methyl radicals, etc. was discussed in details. A pathway diagram of a typical methane combustion process under high temperature condition based on their study is shown in Fig 2.2 (Turns Stephen, 2000). The practice test for real combustion problems with the developed kinetics was also covered in the work. A detailed mecha-

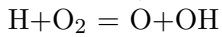
nism with around 255 reactions was presented for hydrocarbon oxidation in the work by Charles Westbrook and Frederick Dryer (Westbrook and Dryer, 1984). Further research on natural gas had shown an addition of small amounts of other hydrocarbons to methane, could result a dramatic increase of energy which is required to ignite the methane as well (Glassman and Yetter, 2008). This feature is relatively important to natural gas combustion, which the majority composition of fuel is methane.

The mechanism for combustion was developed rapidly in 1990s, and there are multiple detailed mechanisms which are available for different operating ranges and different validation methods. One of the most commonly used kinetic mechanism for the natural gas combustion is GRI mechanism (Smith *et al.*, 1999). The newest version of the mechanism which is GRI 3.0 has 325 elementary chemical reactions considering 53 species. Although the mechanism was widely used for different purposes, the attention should be paid as the reaction rates were originally optimized for the temperature range from 1000 K to 2500 K, the pressure range up to 10 atm, and the equivalence ratio from 0.1 to 5. The additional reactions for  $\text{CH}_3\text{O}_2$  and  $\text{C}_2\text{H}_5\text{O}_2$  are needed for a very high pressure or low temperature regions. The  $\text{NO}_x$  production was also considered in the mechanism (Smith *et al.*, 1999).

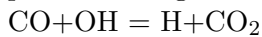
The continuing extension of combustion mechanisms for larger hydrocarbon radicals led to an increased size of kinetic mechanisms (Westbrook *et al.*, 2009). The mechanism was usually developed with the consideration of different reaction classes which may occur under different conditions. A typical kinetic for the high temperature oxidation of n-alkane hydrocarbons contains 9-10 classes as unimolecular fuel decomposition, H-atom abstraction, alkyl radical decomposition, and alkyl radical isomerization (Westbrook *et al.*, 2009). The current developed detailed mechanisms for high-hydrocarbons contain typically more than 1,000 reactions, including approximately 100 chemical species. Therefore the efforts have been made to keep the mechanism small with as much important information could be kept as possible. M.V. Petrova and F.A. Williams (Petrova and Williams, 2006) presented a chemical mechanism which is designed to be used for different fuels for calculating parameters related to autoignition, deflagrations, detonations, and diffusion flames by restricting the application range to a certain value. Another widely used kinetic in combustion research today is

## 2.2. DETAILED KINETICS RESEARCH FOR GASIFIED BIOMASS 17

the San Diego mechanism (Hai Wang, 2007). The mechanism approaches to describe the combustion system and phenomena with minimum number of species and reactions that are required. The mechanism was reported to be able to work with subsets of nitrogen chemistry, JP10 chemistry or Heptane Chemistry for different purpose of researches. Although the detailed mechanisms for specific radicals are constantly developing, most of the time, the combustion rates are only determined by relatively small subsets of elementary reactions through the sensitivity analysis(Androulakis, 2000). The primary chain branching process at high temperature was reported to be the single reaction where the H atom is consumed and O/OH radicals are generated(Westbrook *et al.*, 2005):



The reaction is considered to be essential to the flame propagation, shock tube ignition, detonations and pulse combustors. And the second most sensitive reaction in high temperature combustion is the oxidation of CO which produces a significant amount of heat(Westbrook *et al.*, 2005):



As the mechanisms of hydrocarbon and fossil fuel combustion have been developed for decades since 1950s, there is little effort had been made to the GBG fuel before the 21st century. It is usually considered as same as the intermediate components in other hydrocarbon combustion, and is treated in the same way. One of the major reason for that was relatively few experimental data compare to conventional fuels(Dryer and Chaos, 2008). The large range of the specific composition depending on the fuel source and processing technique is also a reason which made the investigation on GBG fuel combustion a complex task. However, the interests for testing mechanisms for GBG fuels have been increasing in the last decades due to the potential of utilization.

P. Saxena(Saxena and Williams, 2006) tested the mechanism which developed by M.V. Petrova and F.A. Williams(Petrova and Williams, 2006) for the combustion of hydrogen and carbon monoxide, but the purpose of the study was to evaluate the elementary steps for rate parameters modification rather than concern the GBG fuel combustion. Hongyan Sun, etc.(Sun *et al.*, 2007) has measured the laminar flame speed of CO/H<sub>2</sub>/air and CO/H<sub>2</sub>/O<sub>2</sub>/helium respectively, at different mixing ratios as well as a

different equivalence ration. The mechanism for GBG fuel combustion was then developed based on sets of experimental data. The reaction rate constant of  $\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$  was determined and the kinetic model predicted the measured flame speeds and counterflow ignition temperatures accurately. Marcos Chaos and Frederick L. Dryer (Dryer and Chaos, 2008) reviewed the experimental data and kinetic developments for coal-derived syngas (which could be considered as  $\text{H}_2/\text{CO}$  mixture) in gas turbine condition. The impurity coupling combustion with  $\text{NO}_x$  presented in hydrogen fueled system was particularly mentioned by the study. They also found that the hydrogen-oxygen chemical induction processes could be significantly perturbed by nonhomogeneous effects at high pressure and low temperatures which could be a cause inside the gas turbine combustor. D.E. Cavaliere, etc. (Cavaliere *et al.*, 2010) continued the study in coal-derived syngas by evaluating the ignition time to determine the most suitable mechanism for turbine applications. The inability of predicting the performance below 1000 K was reported. It was unsurprised as most of mechanisms were developed only for high temperature combustion. A modified mechanism was developed and reported to have good agreement the experimental data.

## 2.3 Simplified and Reduced Kinetics

Although the detailed kinetics for GBG combustion are developed constantly with recent experimental data, to integrate the detailed chemical kinetics into complex combustion simulations has been proved to be a computationally expensive task. It has been suggested that appropriate simplified kinetics which are computationally efficient could be used instead in complex fluid dynamic models to provide adequate predictions (Jones and Lindstedt, 1988; Abou-Taouk and Eriksson, 2011). The simplified kinetics for specific fuel and operation conditions need to be carefully selected, since they are only valid over limited operating ranges and cannot take account for all of the possible combustion phenomenon.

### 2.3.1 Approaches for Developing Simplified/Reduced Kinetics

There are various approaches for developing simplified/reduced kinetics and new methods are developing constantly. There are generally two major rou-

tines, one is to deduct the required species and reactions for combustion through the analysis of chemical process, and another is to optimize the parameter of reaction rates through a mathematical way. These two major routines were often combined for developing a specific kinetic. Several common approaches are listed here.

- Steady-state approximation. This method assumes the highly reactive intermediate species during the combustion is destroyed as fast as they are formed(Lee *et al.*, 2010). Therefore, these species could be treated as they have reached a steady-state. The method has been developed for a long time(Fraser, 1988) and the advantage of it is there is no need for calculation of reaction rate of these intermediate species. As the intermediated species are usually decided depending on the experiments, the artificial error may occur during the process. New methods which use the computational methods to find the steady-state species are developing in the past twenty years(Jovičić *et al.*, 2008).
- Sensitivity analysis of reaction parameters. The sensitivity analysis determines the effects of uncertainty to the ordinary differential equations (ODEs)(Tomlin *et al.*, 1992). In another word, the sensitivity analysis could provide us the information of which one specific reaction parameter will affect the expected result the most. According to the research, some reaction rate parameters may have minor effects of the specific species concentration. The reaction could be reduced from the complex reaction system to simplify the mechanism. Special focuses need to be paid as the reaction parameter which has minor effect on the specific character of combustion may have a major effect to another character as mentioned in many studies(Petersen *et al.*, 2007a). Therefore the sensitivity analysis has to put all the characters into consideration and attention is needed to use them for untested situations.
- Algorithm methods. The process of using algorithm methods for reducing complex mechanism is based on the mathematical study of reaction rate parameters(Androulakis, 2000). One of the algorithm which considered to be efficient and powerful is the genetic algorithms. The method was developed in early 1970s based on the imitation of natural selection process(Polifke *et al.*, 1998). The set of parameters

("genes") which is considered as a "population" of "individuals" undergoes a "selection" process to achieve the "fittest individuals" of the generation to evolve. The genetic information is exchanged among the parental generation and the random mutations occur with the production of the next generation. Fig 2.3 shows a typical flow diagram for the genetic algorithm. The method has been widely used in various areas and has been reported to be efficient for problems with nonlinear regression.

- Computational singular perturbation (CSP). The method is relatively new and the idea of the method is generally quite similar to the method of steady-state analysis but with the time scale analysis is done dynamically (Massias *et al.*, 1999). The reduced mechanism is therefore more accurate than steady state analysis, due to the species and reactions that can be reduced may change with the reaction progress. The method is also more computationally expensive.
- Intrinsic low-dimensional manifolds (ILDM). The local Jacobian is analysed and which of it correspond to the slowest time scales is used to establish the intrinsic lower dimensional manifold (Gicquel *et al.*, 2000; Fiorina *et al.*, 2003). The system is reported to evolve quickly driven by the fast variables and the dynamics of these variables with slow manifold provides an accurate approximation of the system. The method needs to be preprocessed before it can be used for combustion modelling to generate a lookup-table for the slow variables.

### 2.3.2 Simplified Kinetics for Hydrocarbon/GBG Fuels

Westbrook and Dryer derived 1- and 2- steps simplified reaction kinetics for hydrocarbon fuels and are widely used in the simulation of industrial combustors (Westbrook and Dryer, 1984). Another well-known simplified kinetic is developed by Jones and Lindstedt with 4-step simplified reaction by including two reactions for hydrocarbon oxidation (Jones and Lindstedt, 1988).

In the past decade, there has been attempts to develop simplified kinetics for GBG fuels to fulfil the requirement of CFD simulation. The simplified reaction kinetics from Westbrook-Dryer and Jones-Lindstedt are optimized by A. Cuoci *et al.* (Frassoldati *et al.*, 2009) with comparison to a detailed kinetic in laminar diffusive counter-flow flames.

P. Boivin et al.(Boivin *et al.*, 2013, 2011; Boivin, 2011) developed a four-step reduced mechanism for syngas (CO/H<sub>2</sub>) combustion based on Quasi-Steady State Approximation (QSSA). The kinetic was tested with detailed kinetics and experimental data under various conditions. A moderate agreement is achieved between the detailed kinetic and the reduced version. However, the modifications are needed to achieve better agreements between kinetic calculations and experimental measurements. A syngas burner for gas turbines is simulated in the CFD program by Abdallah Abou-Taouk(Abou-Taouk and Eriksson, 2011; Abou-Taouk *et al.*, 2013) with the reaction kinetics which were optimized for methane-air combustion and syngas-air combustion respectively.





## Chapter 3

# Numerical Models for Combustion Reactions

There are two numerical models are carried out in current work to study the laminar flame speed and ignition delay time of the GBG fuel combustion respectively. A constant volume reactor is used for predicting the ignition delay time of the GBG fuel, and the 1-D laminar premixed flame model is set up for predicting the laminar flame speed. These numerical models are briefly introduced in current chapter with their theoretical laws.

### 3.1 Constant Volume Reactor

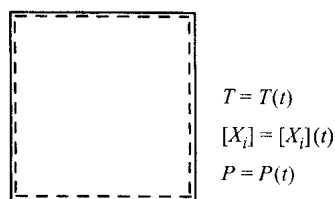


Figure 3.1: Perfectly mixed, homogeneous reactor with constant volume. (Turns Stephen, 2000)

The constant volume reactor model is used to simulate the reaction process of premixed GBG fuel and air with the assumption of adiabatic process

and ideal-gas equation. The condition of the reactor is shown in Figure 3.1(Turns Stephen, 2000). The conservation of energy for the system is:

$$\frac{\dot{Q}}{m} = \frac{du}{dt} \quad (3.1)$$

where  $\dot{Q}$  is the heat flux of the system,  $m$  is the mass,  $u$  and  $t$  represent the internal energy and time respectively. For ideal gases, the equation could be further derived as:

$$\frac{dT}{dt} = \frac{(\dot{Q}/V) - \sum_i (\bar{u}_i \dot{\omega}_i)}{\sum_i (X_i c_{v,i})} \quad (3.2)$$

where  $T$  is the temperature,  $V$  is the volume,  $R_u$  is the universal gas constant,  $\dot{\omega}_i$ ,  $u_i$ ,  $X_i$  and  $c_{v,i}$  represent the production rate, internal energy, mole fraction and constant-volume specific heat of  $i$ th species respectively. Due to the adiabatic assumption in current study,  $\dot{Q}/V = 0$ . The pressure variation rate can be achieved with the differentiate of the ideal-gas law as:

$$P = \sum_i X_i R_u T \quad (3.3)$$

and

$$\frac{dP}{dt} = R_u T \sum_i \dot{\omega}_i + R_u \sum_i X_i \frac{dT}{dt} \quad (3.4)$$

where  $P$  is the pressure of the reaction system. The 3.2 is integrated with the chemical reaction rate from Arrhenius equation to solve the temperature variation and mole fraction variation of specific species:

$$\frac{dT}{dt} = f(X_i, T) \quad (3.5)$$

$$\frac{dX_i}{dt} = f(X_i, T) \quad i = 1, 2, \dots, N \quad (3.6)$$

The integration is normally carried with a stiff equation in the simulation process.

## 3.2 1-D Laminar Premixed Flame

The propagation of a flame is usually a combination effort of heat transfer and mass transportation. The main purpose of the laminar flame model is to study the structure of the premixed flame with the consideration of temperature and composition distribution along the axis. The 1-D adiabatic premixed flame is carried out to achieve this purpose and its typical structure is shown in Figure 3.2.

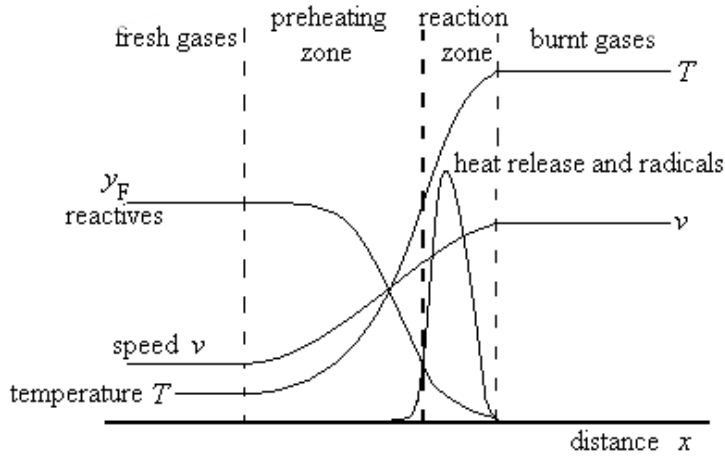


Figure 3.2: Typical structure of 1-D laminar premixed flame.

### 3.2.1 The Governing Equations and Boundary Conditions

The governing equations of the system is achieved when the influence from viscosity effect, body force and heat radiation can be ignored:

Mass Conservation:

$$\dot{m} = \rho v = \text{const} \quad (3.7)$$

Energy Conservation:

$$c_p \dot{m} \frac{dT}{dx} - \frac{d}{dx} \left( \lambda \frac{dT}{dx} \right) + \sum_i \rho Y_i \mathcal{D}_i c_{p,i} \frac{dT}{dx} + \sum_i \dot{\omega}_i \Delta H_i = 0 \quad (3.8)$$

Components Transportation:

$$\dot{m} \frac{dY_i}{dx} + \frac{d}{dx}(\rho Y_i \mathcal{D}_i) - \dot{\omega}_i = 0 \quad i = 1, 2, \dots, N \quad (3.9)$$

where  $\dot{m}$  is the mass flux,  $\rho$  represents the density,  $v$  is the average velocity,  $x$  represents the spacial distance of the 1-D system,  $\lambda$  and  $c_p$  are the thermal conductivity and constant-pressure specific heat of the mixture.  $Y_i$ ,  $\mathcal{D}_i$  and  $\Delta H$  represent the mass fraction, the binary diffusion coefficient and the specific enthalpy of the  $i$ th species. The boundary conditions of the system are:

$$T_{(-\infty)} = T_u \quad (3.10)$$

$$Y_{k(-\infty)} = Y_{u,i} \quad (3.11)$$

where  $T_u$  is the temperature of unburnt gas mixture, and  $Y_{u,i(\Phi)}$  is the mass fraction of  $i$ th species in the unburnt gas flow. And the thermal and transport condition for the system boundary are:

$$\frac{dT}{dx}(+\infty) = 0 \quad (3.12)$$

$$\frac{dY_i}{dx}(+\infty) = 0 \quad (3.13)$$

$\dot{m}$  is unknown in the free propagation flame system, and is considered as Eigenvalues for the boundary condition listed above:

$$\frac{d\dot{m}}{dx} = 0 \quad (3.14)$$

Initial temperature  $T_i$  is set at position  $x = 0$  and the assumption is made that  $T_i$  is small enough that the reaction rate around  $x = 0$  can be ignored to achieve the boundary condition at  $x = 0$ :

$$\dot{m}Y_{i(0)} + \rho_{(0)} + Y_{i(0)}V_{i(0)} = \dot{m}Y_{u,i} \quad i = 1, 2, \dots, N \quad (3.15)$$

The governing equations from 3.7 to 3.11 are combined with boundary conditions 3.12 to 3.15, and the hybrid Newton/time-step algorithm is used to calculate the finite-difference flow equations. To simplify the governing equations, a dimensionless number is defined as the ratio of thermal diffusivity and mass to mass diffusivity, which is called Lewis number:

$$Le_i = \frac{\lambda}{\rho D_i c_p} \quad (3.16)$$

where  $D_i$  is the mass diffusivity of  $i$ th species in the mixture.

### 3.2.2 Numerical Solution of Governing Equations

As already mentioned in previous sections, the numerical methods which are used to solve governing equations of the 1-D flame system is the finite-difference equation. The approximate solutions are achieved for governing equations on finite elements in the concerned region. The length of the region is set to be long enough so that the gradients of concentration and temperature can be considered as 0 at the position  $x = L$ .

The second order derivative in the governing equations is solved by second-order central difference, while the first-order derivative is solved by first-order upwind difference. The diffusion and the multi-components effects are put into concern. The finite-difference equations are written in a residual form.

$$F(\Phi) = 0 \quad (3.17)$$

where the function  $F$  is the finite-difference form of the governing equations and boundary layers on the grid point, and  $\Phi$  represents the solution vector. The residual equations are solved by a variant of Newton's methods: Linearize solution estimate the value of  $\Phi^{(0)}$ :

$$F_{lin,k}^{(0)} = F_k(\Phi^{(0)}) + \sum_j \left. \frac{\partial F_i}{\partial \Phi_j} \right|_{\Phi=\Phi^{(0)}} (\Phi_j - \Phi_j^{(0)}) \quad (3.18)$$

where  $k$  and  $j$  represents the  $k$ th equation and  $j$ th point in the domain respectively. The new estimates of  $\Phi$  is solved with following equations:

$$F_{lin}(\Phi^{(1)}) = 0, \quad (3.19)$$

$$\Phi^{(1)} = \Phi^{(0)} - [J^{(0)}]^{-1} F^{(0)} \quad (3.20)$$

where  $J$  is the Jacobian matrix of the system. Therefore, the iteration is carried out with a general expression as:

$$J(\Phi^{(n)})(\Phi^{(n+1)} - \Phi^{(n)}) = -\psi^{(n)} F(\Phi^{(n)}) \quad n = 1, 2, 3, \dots \quad (3.21)$$

where  $\psi(0 < \psi \leq 1)$  is the relaxation factor of  $n$ th iteration. The iteration is considered as converged when  $|\Phi^{(n+1)} - \Phi^{(n)}|$  and  $|F(\Phi^{(n)})|$  reach the tolerance value. Moreover, a good estimation is required for  $\Phi^{(0)}$  to reach the convergence. The selection of  $J^{(n)}$  and relaxation factor  $\psi^{(n)}$  is controlled to satisfy the relation:

$$|(J^{(n)})^{-1} F(\Phi^{(n+1)})| < |(J^{(n)})^{-1} F(\Phi^{(n)})| \quad (3.22)$$

The relation equation decreases the converge speed, but ensure the iteration results are limited in a correct range.

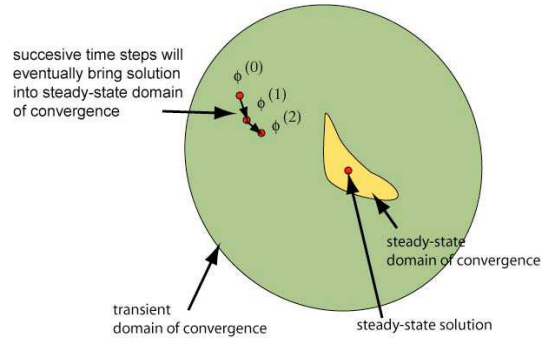


Figure 3.3: The larger convergence domain for the hybrid Newton/transient method.

However, due to the high-order nonlinear terms present with reaction kinetics, the equation 3.17 is unstable under certain circumstance and the steady-state solution cannot be reached. The pseudo-transient problem is solved with a larger domain to achieve the convergence. It is constructed by adding transient terms into conservation equations. The new equation is described as:

$$F_{tr}(\Phi^{(n+1)}, \Phi^{(n)}, \Delta t) = 0 \quad (3.23)$$

The procedure of transient calculation is shown in 3.3. The hybrid method generally tries to solve steady-state problem with certain time steps. If the convergence cannot be reached, more time-steps will be taken with sufficiently small time steps where the transient residual function can be considered as a linear problem. The process is repeated until steady-state Newton method is succeeded to converge.

## Chapter 4

# Kinetic Study of GBG Fuel Combustion

This chapter will discuss the kinetic study of the GBG fuel combustion based on the published results in Paper 1, 2 and 3. Additional research progress is also presented here related to the chemical kinetic studies. The kinetic study of the chemistry kinetic is important for understanding the fundamental of the combustion process and for prediction of the flow field distribution. The appropriate kinetics are still required to reproduce the chemical reaction process and the species transportation.

### 4.1 Approach for Kinetic Study

The kinetic studies which are included in current work are aimed to study the combustion features of GBG fuels through numerical simulations. The simulation results and experimental data are compared with the results from methane combustion and also with each other. In Chapter 2 which describes the progress of chemistry kinetic study, both detailed and simplified kinetics are mentioned. The kinetics from both types will be evaluated here. For the conditions which experimental data are hard to achieve, the evaluation bases on the comparison of simplified kinetic to detailed kinetics.

### 4.1.1 Gas Mixtures

In the process of biomass gasification, the specific composition of GBG fuels could vary in a wide range. A typical GBG fuels consist preliminary of  $H_2$  and  $CO$  as combustible substance(Zhang *et al.*, 2013; Munajat *et al.*, 2012; Cheng *et al.*, 2011; ?; Narvaez *et al.*, 1996; Hanaoka *et al.*, 2005), with the presence of small amounts of  $CH_4$  and other higher hydrocarbons. It may often contain other diluent gases such as  $O_2$ ,  $CO_2$  and  $H_2O$ . However, the specific composition of the fuel varies due to the biomass source and the processing methods(Serrano *et al.*, 2008; Vu *et al.*, 2011; Liu *et al.*, 2010).

For all the experiments related to GBG gas combustion in the study, a simulated gas mixture is used to present the real GBG fuels. By using the  $CO/H_2/CH_4/CO_2$  and  $O_2$  mixture, it contains the main components of a typical GBG fuel and could be controlled by a mass flow rate to mix with air. Water vapour is introduced with different concentration to evaluate the effect. Furthermore, the experimental data from other studies are also extracted for comparison and validation. The major gas mixture with their compositions are listed in Table 4.1. The uncertainty of mixture is estimated from  $\pm 1.1\%$  to  $\pm 1.3\%$  in volume for the current experiment.

### 4.1.2 Premixed Burner for Kinetic Study

To study the basic features of the GBG fuel combustion, a simple burner stabilized flame was used in previous studies and the GBG fuels are premixed with air before entering the burner. The laminar speed was extracted as the key feature to be studied for the GBG fuel combustion as it is one of the essential parameters. It contains relative information on reactivity, diffusivity and exothermicity and is widely used for validating reaction dynamic models. For practical reason, the laminar flame speed as a indicate is used for predicting flashback, blow off, flame stability and propagation.

The basic experimental setup of the premixed burner is shown in Figure 4.1(Zhang *et al.*, 2013). A mixture of  $CO/H_2/CH_4/CO_2$  with specific concentrations and  $O_2$  is initially contained in two bottles respectively. And they are then rapidly mixed through a mixing panel. The mixture is controlled and measured by mass flow controllers (MFC) as well as the air flow. They are mixed before entering the burner. The liquid water is injected precisely via a syringe pump into the heated fuel mixture stream.



Table 4.1: Gas components of different GBG fuel mixture.

| GBG Fuel Composition [% in volume] |                |                 |                 |                |                  |  | LHV ( $MJ/m^3$ ) |
|------------------------------------|----------------|-----------------|-----------------|----------------|------------------|--|------------------|
| CO                                 | H <sub>2</sub> | CH <sub>4</sub> | CO <sub>2</sub> | O <sub>2</sub> | H <sub>2</sub> O | Others   |                  |
| Current Study                      |                |                 |                 |                |                  |  |                  |
| 23.75-25                           | 12-12.5        | 2.4-2.5         | 9.5-10          | 47.5-50        | 0-5              | $T_{int}^*$  | 5.13-5.4         |
| Wood Syngas                        |                |                 |                 |                |                  |  |                  |
| 14.24                              | 10.68          | 3.54            | 14.18           | 55.2           | 0                | C <sub>2</sub> H <sub>4</sub> ,<br>C <sub>2</sub> H <sub>6</sub> | 4.95             |
| Clean Syngas                       |                |                 |                 |                |                  |  |                  |
| 19                                 | 12             | 5.8             | 13.2            | 50             | 0                | 0  | 5.78             |
| 21-24                              | 11-17          | 0-3             | 9-13            | 48-53          | 0                | 0  | 4.84-5.29        |

\* The current study includes the effect of inlet temperature change of GBG mixture.

A set of Xenon lamp, lenses and mirrors are used for generating Schlieren images of the flame. The laminar flame speed is then calculated through the mass conservation balance equation:

$$S_L = \frac{\dot{m}}{\rho_u A_b} = \frac{\dot{\mu}}{A_b}, \quad (4.1)$$

where  $\dot{\mu}$  is the volumetric flow rate and  $A_b$  is the area of flame reaction zone, which is determined by the Schlieren image.

To validate the kinetic model with a certain range, various sets of operating conditions are selected for experiments. The equivalence ratio of the fuel-air mixture varies from 0.95-1.3 and the initial temperature is varied from 298 K to 423 K. For the mixture has lower or higher equivalence ratio, it has difficulty to be stabilized on current experimental setup.

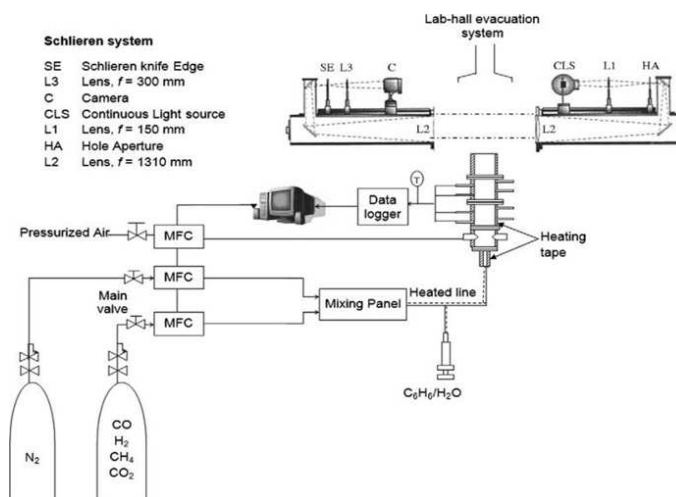


Figure 4.1: Perfectly mixed, homogeneous reactor with constant volume. (Zhang *et al.*, 2013)

### 4.1.3 Kinetics Used in Current Study

Three sets of Detailed kinetics are chosen to evaluate the combustion features of GBG fuels. GRI3.0 (Smith *et al.*, 1999) is an optimized mechanism originally designed to model natural gas combustion with NO formation and recombust chemistry. It contains totally 325 reactions and 53 species. San Diego mechanism (Mechanical and Aerospace Engineering Combustion Research, 2014) contains 235 reactions and 38 species are also developed for natural gas combustion and widely used for kinetic optimization. Finally, the kinetic which developed by University of Southern California (Hai Wang, 2007) for combustion reaction of  $H_2/CO/C1-C4$  compounds are selected with the largest number of reactions in current study – which contains 784 reactions and 111 species.

Furthermore, several sets of simplified chemical kinetics are chosen to be evaluated and optimized with the experimental data and numerical results from detailed kinetics. The original and developed kinetic sets (WD kinetics) based on the study of Westbrook and Dryer (Westbrook and Dryer, 1984) are presented 4.2 with reactions R1 and R2, while another set (LJ kinetics) based on the study of Jones and Lindstedt (Jones and Lindstedt,

Table 4.2: Reaction rate equations and parameters from Westbrook-Dryer kinetics.

| <i>No.</i> | <i>Reactions</i>  | <i>A</i>               | <i>β</i> | <i>E<sub>A</sub></i> | <i>Reaction Orders</i>                                     |
|------------|---|------------------------|----------|----------------------|--|
| R1         | $\text{CH}_4 + 1.5\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2\text{O}$ | $1.590 \times 10^{13}$ | 0        | 47800                | $[\text{CH}_4]^{0.7}[\text{O}_2]^{0.8}$                    |
| R2         | $\text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2$                       | $3.980 \times 10^{14}$ | 0        | 40700                | $[\text{CO}][\text{O}_2]^{0.25}[\text{H}_2\text{O}]^{0.5}$ |
| R2r        | $\text{CO}_2 \rightarrow \text{CO} + 0.5\text{O}_2$                       | $5.000 \times 10^8$    | 0        | 40700                | $[\text{CO}_2]$  |
| R3         | $\text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O}$               | $9.870 \times 10^{11}$ | 0        | 7400                 | $[\text{H}_2][\text{O}_2]$                                 |
| R4         | $\text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2$                       | $4.090 \times 10^{13}$ | 0        | 31700                | $[\text{CO}][\text{O}_2]^{0.25}[\text{H}_2\text{O}]^{0.5}$ |
| R4r        | $\text{CO}_2 \rightarrow \text{CO} + 0.5\text{O}_2$                       | $4.450 \times 10^9$    | 0        | 41300                | $[\text{CO}_2]$  |
| R5         | $\text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O}$               | $1.097 \times 10^{11}$ | 0        | 6900                 | $[\text{H}_2]^{0.87}[\text{O}_2]^{1.10}$                   |
| R6         | $\text{CH}_4 + 1.5\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2\text{O}$ | $1.400 \times 10^{10}$ | -0.062   | 27900                | $[\text{CH}_4]^{0.5}[\text{O}_2]^{1.066}$                  |
| R7         | $\text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2$                       | $7.380 \times 10^{11}$ | 0.215    | 18300                | $[\text{CO}_2][\text{O}_2]^{0.5}$                          |

1988) is presented in 4.3 with reactions R8 – R11. These two sets of simplified kinetics are commonly used for the numerical study of natural gas combustion under industrial conditions, and they were originally developed by the research of high temperature oxidation reactions with lean turbulent combustion and by studying premixed and non-premixed flames of alkane hydrocarbons respectively. As the CO/H<sub>2</sub> mixture oxidation is often dominant in most GBG fuel combustion, several sets derived and optimized from original WD kinetic and LJ kinetic are also listed 4.2 and 4.3. The detailed description of reactions is included in Paper 1.

## 4.2 Results and Discussion

The characteristic study of GBG fuel with the concern of laminar flame speed and ignition delay time is carried out using the kinetic models and the experimental data from previously published papers. The main conclusions are presented here.

Table 4.3: Reaction rate equations and parameters from Jones-Lindstedt Kinetic.

| <i>No.</i> | <i>Reactions</i>  | <i>A</i>               | <i>β</i> | <i>E<sub>A</sub></i> | <i>Reaction Orders</i>                                 |
|------------|---|------------------------|----------|----------------------|--|
| R8         | $\text{CH}_4 + 0.5\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2$         | $7.820 \times 10^{13}$ | 0        | 30000                | $[\text{CH}_4]^{0.5}[\text{O}_2]^{1.25}$               |
| R9         | $\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$    | $3.000 \times 10^{11}$ | 0        | 30000                | $[\text{CH}_4][\text{H}_2\text{O}]$                    |
| R10        | $\text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O}$               | $1.209 \times 10^{18}$ | -1       | 40000                | $[\text{H}_2]^{0.25}[\text{O}_2]^{1.5}$                |
| R10r       | $\text{H}_2\text{O} \rightarrow \text{H}_2 + 0.5\text{O}_2$               | $7.060 \times 10^{17}$ | -0.870   | 97900                | $[\text{H}_2]^{-0.75}[\text{O}_2][\text{H}_2\text{O}]$ |
| R11        | $\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2$ | $2.750 \times 10^{12}$ | 0        | 20000                | $[\text{CO}][\text{H}_2\text{O}]$                      |
| R12        | $\text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O}$               | $1.050 \times 10^{17}$ | -1       | 37700                | $[\text{H}_2]^{0.33}[\text{O}_2]^{1.4}$                |
| R12r       | $\text{H}_2\text{O} \rightarrow \text{H}_2 + 0.5\text{O}_2$               | $6.020 \times 10^{18}$ | -0.870   | 94000                | $[\text{H}_2]^{-0.75}[\text{O}_2][\text{H}_2\text{O}]$ |
| R13        | $\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2$ | $2.630 \times 10^{13}$ | 0        | 18500                | $[\text{CO}][\text{H}_2\text{O}]$                      |

#### 4.2.1 The study on kinetic evaluation of laminar flame speed (Paper 2)

- The calculated results of the laminar flame speed from chemical mechanisms have shown a generally good agreement with the experimental measurements under fuel-lean condition and with an initial temperature of 298 K at atmospheric pressure. However, the calculated results for fuel-rich conditions and increased initial temperature or pressure have shown deviations from experimental data. The deviation for simulated GBG fuel (with a mole fraction: 25% of CO, 12.5% of H<sub>2</sub>, 10 % of CO<sub>2</sub>, 2.5% of CH<sub>4</sub> and 50 % of O<sub>2</sub>) which is used in the current study and the initial temperature at 398 K is 20% to 30% with different equivalence ratio and detailed mechanisms. The deviation also appeared with higher hydrogen levels at fuel-rich condition. A sensitivity analysis based on the simulated GBG fuel suggests a potential refinement of existing mechanisms is needed for the reactions  $\text{H} + \text{O}_2 = \text{O} + \text{OH}$  and  $\text{H} + \text{CH}_3 (+\text{M}) = \text{CH}_4 (+\text{M})$  under fuel-rich conditions at a higher initial temperature.
- The increased initial temperature has shown an effect of increasing laminar flame speed for biomass derived fuels in the current study for temperature up to 398 K.

- On the other hand, the increased pressure has an effect of reducing laminar flame speed for biomass derived fuels. A detailed study of the effects of temperature and pressure for specific fuels with a certain equivalence ratio suggests that the empirical relationship derived from previous work has a good agreement with the experimental data.
- Furthermore, a set of empirical equations has been developed for predicting laminar flame speeds of current GBG fuel over a range of initial temperature from 298 to 398 K and pressure from 1 atm to 10 atm. The empirical equation of laminar flame speed for current GBG fuel composition is given as:

$$S_L = S_L^0 \left(\frac{T_u}{T_0}\right)^\alpha \left(\frac{P_u}{P_0}\right)^\theta \quad (4.2)$$

where  $S_L^0$ ,  $T_0$  and  $P_0$  are the reference value of laminar flame speed, temperature and pressure respectively. The coefficients  $\alpha$  and  $\theta$  for the GBG fuel can be expressed as a function of the equivalence ration  $\phi$ :

$$\alpha = -0.287\phi^2 + 0.716\phi + 1.51 \quad (4.3)$$

$$\theta = -1.36\phi^2 + 2.989\phi - 2 \quad (4.4)$$

- Among the variety of fuel compositions, the concentration of  $H_2$  in the biomass derived fuels has shown dominant influence for the laminar flame speed variation. However, it should be careful to deduce the laminar flame speed directly from  $H_2$  concentration, especially with the very rich mixture combustion. CO concentration also has effects on laminar flame speed, but the effects is not as significant as  $H_2$  concentration.
- Hydrocarbons like  $CH_4$  also have an effect on the laminar flame speed of biomass derived fuels. The most significant change that discovered in the current study is the shift of peak laminar flame speed and the decrease of laminar flame speed with fuel-rich combustion. The diluents at the same time also have a significant effect on the laminar flame speed of selected compositions.

### 4.2.2 Numerical study on ignition delay time (Paper 3)

- The ignition delay time of the current GBG fuel is calculated under various pressures (1 atm, 4 atm, 16 atm and 32 atm) using GRI 3.0 mechanism, San Diego mechanism and a simplified mechanism developed by Ranzi et al. for CO/H<sub>2</sub> mixture. A general agreement was reached with different mechanisms. However, a deviation was discovered for the mechanism scheme from Ranzi et al.'s research. The deviation is considered mainly caused by the ignorance of CH<sub>4</sub> in mechanism schemes. The same set of mechanisms was used for numerical calculation of ignition delay time for a CO/H<sub>2</sub>/air mixture and a CO/H<sub>2</sub>/CO<sub>2</sub>/air mixture from previous studies of Kalitan et al. (Kalitan *et al.*, 2007, 2006) and Petersen et al. (Petersen *et al.*, 2007a,b) respectively. The numerical results obtained in this study have been compared with the experimental data published by these researches. A best agreement was achieved for CO/H<sub>2</sub>/air mixture under the pressure of 15.4 atm which the full transition of the H<sub>2</sub> oxidation system to the second explosion limit was completed. The calculation results under 1.1 atm and 2.5 atm overestimated the ignition delay time of similar mixture. The deviation was more significant with low-temperature regime (900 K < T < 1000 K) under 2.5 atm due to a failure of capturing the transition of H + O<sub>2</sub> reaction from chain-branching to chain-terminating. The deviation was also observed for CO/H<sub>2</sub>/CO<sub>2</sub>/air mixture at the lower - temperature regime and possible explanations were discussed.
- The calculated ignition delay time of current GBG fuel was then evaluated with a temperature range from 900 K to 1250 K and a pressure range from 1 atm to 32 atm. The results were carried out with equivalence ratios at 0.5, 1 and 2. Different behaviours were observed with an increased pressure for high temperature regime (1150 K < T < 1250 K) and low temperature regime (900 K < T < 1050 K) respectively. There was no unified correlation between the ignition delay and pressure through the range. However, a general correlation could be established in the pressure range of 8 – 32 atm with a factor of. The correlation of ignition delay time and temperature was more significant with a factor of  $\exp(20095 \pm 130/T)$  for the range of 900 – 1250 K. The numerical results of ignition delay time for a CO/H<sub>2</sub>/O<sub>2</sub>/Ar mix-

ture were also carried out and compared with experimental data from the previous study of Keromnes et al. (Kéromnès *et al.*, 2013). As the numerical calculation had shown a good agreement with experimental data, a regression analysis of the experimental data gave an empirical equation as  $\tau_{ign} = 8.5 \times 10^{-3} \exp(3.7 \times 10^6 / T^{1.5}) P^{0.7}$ .

- A further study of ignition delay time for current GBG fuel was done by considering the influence of equivalence ratio. Different behaviours of ignition delay time again observed with different temperature regimes and different pressure regimes and led to a complex equation. For a pressure range of 8 – 32 atm, a general correlation equation was proposed for current GBG fuel as  $\tau_{ign} = 4.6 \times 10^{-5} \exp(20095 \pm 130/T) P^{-0.5 \pm 0.03} \phi^{-0.31 \pm 0.03}$ .
- The influence of fuel composition was discussed in the final part of current research. The calculated results of the CO/H<sub>2</sub>/CO<sub>2</sub>/CH<sub>4</sub>/N<sub>2</sub>/air mixture had shown a slight decrease in ignition delay time with an increased CO concentration, and the similar trend was discovered for an increased H<sub>2</sub> concentration. However, these influences were not significant and were not observed with experimental data from various gas compositions.

### 4.3 Evaluation and optimization of the Kinetics for GBG Fuel Combustion

The evaluation of two different detailed kinetics and several simplified kinetics for GBG fuel combustion is carried in Paper 1. The results show slightly over-estimation of laminar flame speed when use detailed kinetics for current experimental cases. However, the comparison with other experimental data shows different behaviours. Some of them were slightly over-estimated, while others were generally accurate. The simplified kinetics which use the global reaction scheme are failed to predict the laminar flame speed of GBG combustion, and shows a requirement to be optimized before using them in the combustion simulation.

To extend our evaluation from Paper 1. Different detailed kinetics are compared in Figure 4.2. For the experimental data, the statistically fitted equation for predicting laminar flame speed from Monteiro et al. (Monteiro *et*

*al.*, 2010) work is chosen. The equation was developed from the experimental data of an updraft syngas with an equivalent ratio from 0.9 to 1.3. Among

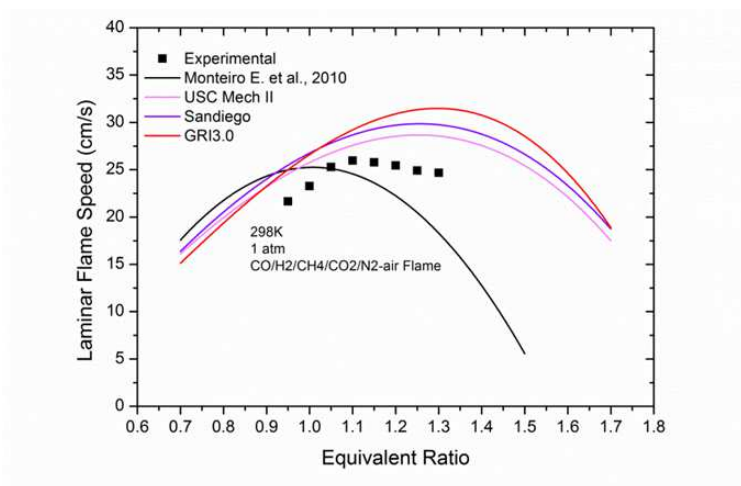


Figure 4.2: Laminar Flame Speed predictions using different kinetics compared with experimental data.

all the detailed kinetics, they have almost similar trends for laminar flame speed prediction. However, The prediction results from the USC Mech II shows the best estimation when compared with experimental results. At the same time, three kinetics all have an overestimation of laminar flame speed which may due to the adiabatic assumption in the simulation process. The statistical equation from Monteiro E. et, al.(Monteiro *et al.*, 2010) study has a reasonable agreement with detailed kinetics for the equivalent ratio lower than 1.0, but the derivation occurs when moving towards the fuel-rich region.

The sensitivity analysis is carried out with the stoichiometry mixture and the most important reactions are listed in Figure 4.3 with their normalized sensitivity of flow rate to pre-exponential rate constants. The sensitivity calculated from three different detailed kinetic mechanisms is shown here. To unify the reactions for comparison, the reactions from GRI 3.0 mechanism are used here. Some of these reactions may take several steps in other kinetics, and therefore a combined sensitivity is used here to evaluate the importance. As it is shown in Figure 4.3, almost same sets of



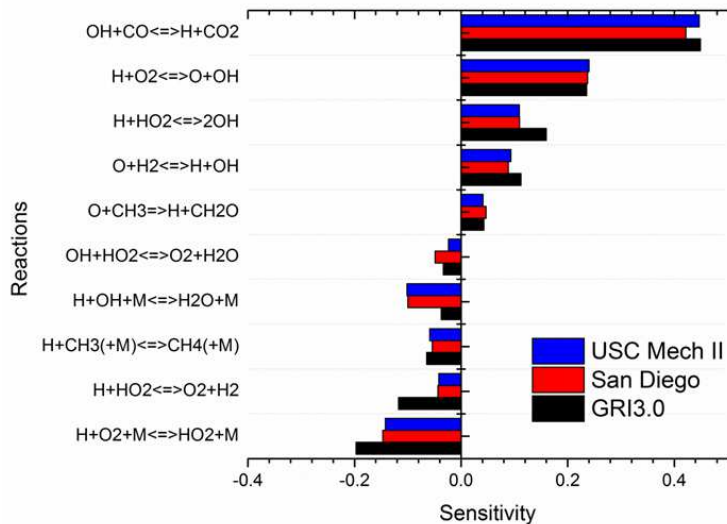


Figure 4.3: Normalized sensitivities of flow rate to pre-exponential rate constants for most important reactions calculated for GBG fuel and air mixture of stoichiometry.

most important reactions are found for different kinetics. The reactions of  $\text{OH} + \text{CO} \leftrightarrow \text{H} + \text{CO}_2$ ,  $\text{H} + \text{O}_2 \leftrightarrow \text{O} + \text{OH}$  and  $\text{H} + \text{O}_2 + \text{M} \leftrightarrow \text{HO}_2 + \text{M}$  are considered to be the most sensitive reactions in the current study. The most important  $\text{OH} + \text{CO} \leftrightarrow \text{H} + \text{CO}_2$  has been discussed in the former research by Chaos and Dryer and is stated of essential in oxidation of  $\text{CO}/\text{H}_2/\text{O}_2$  system as well as the moist  $\text{CO}$  mixture. There is also a suggestion that the reactions involving  $\text{H}$  atom and  $\text{OH}$  radical needs further investigation for better estimation of the laminar flame speed of the  $\text{H}_2/\text{CO}$  mixture with fuel-rich conditions.

The optimization of simplified kinetics based on LJ kinetic is also carried out in Paper 1 and an optimized version of kinetic is developed based on JL mechanism. The reactions which include in the optimized kinetic is listed in Table 4.4 The comparison between the numerical calculation of optimized kinetic and experimental data has shown a relatively good agreement with a certain extension of inlet temperature and equivalence ratios for current GBG fuels. The comparison between the numerical results from optimized

Table 4.4: Optimized kinetic sets for GBG/air combustion

| <i>No.</i> | <i>Reactions</i>  |
|------------|---|
| O1         | $\text{CH}_4 + 0.5\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2$         |
| O2         | $\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$    |
| O3         | $\text{H}_2 + 0.5\text{O}_2 \leftrightarrow \text{H}_2\text{O}$           |
| O4         | $\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2$ |
| O5         | $\text{O}_2 \leftrightarrow 2\text{O}$                                    |
| O6         | $\text{H}_2\text{O} \leftrightarrow \text{H} + \text{OH}$                 |

simplified kinetic and detailed kinetics has also shown a certain agreement with each other with water vapor injections.

## Chapter 5

# Conclusions and Future Prospects

### 5.1 Conclusions

The current study on the combustion features of GBG fuels is carried out based on the numerical calculations. It is considered as a fundamental to understand the combustion system which can handle the GBG fuels in an efficient way. Furthermore, the numerical model and chemical kinetics structured in current work is expected to be used as a first step to develop the combustion simulation method for complex combustion processes of GBG fuels.

As the flexible combustion system is preferred in industrial utilization such as gas turbine combustor or internal combustion engine, a wide range of compositions based on the gasification process of biomass is selected in the research. The variation of the operating condition is also considered in current work with sets of initial temperatures, pressures and equivalence ratios for laminar flame speed and ignition delay time respectively. Due to the lack of relevant experimental studies on GBG fuels with a wide range of conditions, the results from the numerical study can be added to existing database as a supplement, while the empirical relations achieved can be used to guide the experimental set-ups and computational fluid dynamic models.

Some of the brief conclusions from the current study are listed as follow:

- The numerical methods established using chemical kinetics are used to predict the combustion features for GBG fuels. The constant-volume reactor and 1-D flame model are used to calculate the ignition delay time and the laminar flame speed respectively. Several sets of detailed chemical mechanisms were selected in the study, and reasonable agreement is reached between the results from different mechanisms for both laminar flame speed calculation and ignition delay time calculation.
- For the evaluation of laminar flame speed presented in Paper 2, the calculated results from chemical mechanisms has shown a good agreement with experimental data with fuel-lean condition and lower initial temperature. The derivations are found with fuel-rich and increased initial temperatures, as well as the increased pressures. However, the increase of initial temperature has a general trend to increase the laminar flame speed, while the increase of pressure has trend to decrease the laminar flame speed. For the gas composition variation, the H<sub>2</sub> concentration has shown a dominant effect on laminar flame speed while other components are also hard to be ignored. The empirical equations for current GBG fuel are developed to guide the experimental set-up and numerical simulations.
- The ignition delay times calculated from different chemical mechanisms have shown a general agreement with each other. However, the derivation exists in the low-temperature and low pressure regime when comparing the numerical results with experimental data. The influences of initial temperature and pressures on the ignition delay time of the GBG fuel are discussed in Paper 3, as well as the influence of equivalence ratio of the mixture and the variation of compositions. Empirical equations are also developed in the work.
- To optimize the existing simplified kinetics to be used in the future study of combustion simulation, Paper 1 presents a evaluation and optimization of existing kinetics based on the laminar flame speed for GBG fuel combustion. The simulation results are compared with the experimental data and water vapour is presented in the study as dilute. As the results indicate, the reduced kinetics which are developed

for hydrocarbon or hydrogen combustion need to be optimized before using them for GBG combustion. Further optimization of the reduced kinetics is done for GBG and moderate results are achieved using the optimized kinetics compared with the detailed combustion kinetics.

## 5.2 Future Prospects

As mentioned before, the current work is a fundamental study which helps to better understand the combustion process of GBG fuels. The expectation of the work is to help improving the existing combustion engines to handle the variation of GBG fuels with low heating value. The empirical results are expected to be used as guidelines to build the experimental set-up, and to be used in the simulation model for complex combustion processes. Some of the future prospects can be used to develop current work are listed here:

- The results achieved from the numerical calculations of chemical mechanism should be validated with more experimental data in a wide range of operating conditions. The perspective was actually carried out through the whole study. However, the experimental data is still limited for GBG fuels, especially for the high pressure and low initial temperature cases, which is the operating condition in most industrial combustors. Therefore, more experimental data is required for these conditions with more accurate measurement methods
- A numerical study of complex combustion process should be carried out for the GBG fuel combustion. Influences from the fluid dynamic process should be put into concern with the chemical reaction process, especially for the case when turbulent flow and chemical reaction have interactions with each other. The appropriate method to combine the stiff solver of kinetics with fluid dynamic will be the focus point to look at.
- The combustion features of GBG fuels should be evaluated with more perspectives with the establish of complex combustion system. The features such as turbulent flame surface propagation, turbulent flame structure, combustion stability and flame attacking angle of swirls flame should be put into concern.

- The emission problem is the focus point for combustion engineer as the environmental crisis increases. The emission from the combustion process of GBG fuel should be studied in details. And the influence of operating conditions and equivalence ratios should be done.
- Based on the experimental study and numerical models of GBG fuel combustion. The ultimate goal of the study is to develop the existing combustion process to achieve a more efficient way for GBG fuel utilization. The design and improvement of the burner system can be carried out for instant.

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