Fuel 220 (2018) 283–295

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Full Length Article

An investigation of fuel variability effect on bio-syngas combustion using uncertainty quantification

Kai Zhang, Xi Jiang*

School of Engineering & Materials Science, Queen Mary University of London, Mile End Road, London E1 4NS, UK

A R T I C L E I N F O

Keywords:
Uncertainty quantification
Bio-syngas combustion
Fuel variability
Polynomial chaos expansion
Targeted uncertainty reduction

A B S T R A C T

Fuel variability effects on physicochemical properties such as adiabatic flame temperature and laminar flame speed of premixed bio-syngas combustion are investigated via polynomial chaos expansion (PCE) based uncertainty quantification (UQ) approach at several equivalence ratios. Questions regarding confidence level of using bio-syngas with varying fuel composition are tackled from a statistical point view. Impacts of unburnt gas temperature and different chemical mechanisms (GMI-Mech 3.0 and San Diego Mechanism) on predicted uncertainties of these combustion properties are discussed. It was found that fluctuation of flame temperature at various equivalence ratios is less affected by bio-syngas fuel variabilities, while flame speed is sensitive to uncertainties in fuel composition. For instance, 1.5% fluctuation of bio-syngas constituent can lead to 14% fluctuation of flame speed for rich combustion, and 3% for lean combustion. Less than 0.8% fluctuation of flame temperature due to variability of bio-syngas fuel composition was observed. UQ of bio-syngas combustion showed that hydrogen variability plays a significant role (70–80% at lean condition) in flame speed variation, while methane variability, although thought to be important, has a negligible impact except for fuel-rich combustion. Overall, the current study has provided a fundamental understanding of the effects of fuel variability on physicochemical properties of bio-syngas combustion. Dominating compositions to variations of bio-syngas combustion are provided quantitatively to guide targeted uncertainty reduction from the upstream gasification process.

1. Introduction

Bio-syngas, generated from gasification of CO_2 neutral biomass, is known as a clean and renewable energy source [1]. It has drawn lots of research attentions not only because of an increasing demand of energy worldwide with depleting natural resources, but also because of its versatile use for heat and electricity generation, methanol and hydrogen production *etc.* [2]. Despite its promising prospect [3], bio-syngas is not broadly used mainly because of its complex chemical composition [4]. Depending on means of gasification/production and sources of biomass [5–7], typical bio-syngas consists of 22–32% hydrogen (H_2), 28–36% carbon monoxide (CO), 21–30% carbon dioxide (CO_2), and a small amount of methane 8–11% by volume [1]. The variable fuel composition can cause significant problems in the combustion of bio-syngas in practical systems; unpredictable combustion performance, combustion instability and hot spots may deteriorate and damage the combustion hardware [8]. Minor constituents such as tars and moisture, impurities such as hydrogen cyanide and ammonia in bio-syngas fuel also increase the difficulty of using bio-syngas fuel. To deal with this challenge, an in-depth understanding of combustion performances of bio-syngas concerning the significant uncertain variation of its composition is required.

Over the years, effects of H_2:CH_4 ratio [9,10], nitrogen dilution [11], impurities (such as NH_3, HCN *etc.*) [12,13] or moistures and tars [14,15] and other effects in syngas have been investigated at various operating conditions. Laminar burning velocity of natural gas-hydrogen-air mixtures was measured by Huang et al. [9] in a constant-volume bomb at normal temperature and pressure with correlations for calculating laminar burning velocity of the mixture established based on experimental data. Hu et al. [10] further studied hydrogen enriched methane mixture, and considered three combustion regimes depending on hydrogen fraction in the fuel blend. Laminar burning velocity was seen to increase linearly with the increase of hydrogen fraction when hydrogen fraction is below 60% or above 80%, while exponential dependency was observed for transition regime where hydrogen fraction is between 60% and 80%. Prathap et al. [11] discussed combustion performances of nitrogen diluted syngas. An increase of the proportion of%N_2 by volume from 0 to 60 in syngas (H_2:CO = 1) augments the

* Corresponding author.
E-mail address: xi.jiang@qmul.ac.uk (X. Jiang).

https://doi.org/10.1016/j.fuel.2018.02.007
Received 2 December 2017; Received in revised form 13 January 2018; Accepted 2 February 2018

coupled effect of flame stretch and preferential diffusion on laminar flame speed. Effects of impurities such as NH_3 and HCN were examined by Mathieu et al. [13]. A slight decrease of laminar flame speed of combusting NH_3 and HCN diluted syngas at fuel rich condition is observed, while laminar flame speed is not sensitive to NO_2 addition.

Bio-syngas is generally more complex than other types of syngas generated from hydrocarbon feedstock in terms of composition and combustion performance. Due to the complexities in fuel composition [16–22], many fundamental studies were focused on performances of hydrogen-enriched carbon monoxide combustion imitating main compositions of the fuel mixture. Bhaduri et al. [16] investigated the effect of H_2:CO ratio, moisture, and tars in a HCCI engine at various temperatures and pressures. It was concluded that bio-syngas ignition is delayed by moisture while the effect of tars is insignificant. Sahoo et al. [17] reported that higher H_2:CO ratio results to higher NOx emission because of faster combustion of H_2 in syngas. Ranga Dinesh et al. [20–22] investigated fuel variability effect of hydrogen-enriched carbon monoxide flames at various conditions using large eddy simulation. High diffusivity and reactivity of hydrogen have a large impact on combustion performances such as flame temperature, flame thickness, near wall flame structure, combustion products *etc.* In addition, Fischer and Jiang [23] studied effects of variations in bio-syngas fuel composition on combustion. Sensitivity analyses were performed and led to the finding that kinetic coefficients for reactions involving HO_2 free radial might not be optimally known.

Despite these findings, parametric studies as those mentioned above have only provided guidance on effective use of bio-syngas in a 'set of definite events' since results have offered 'definite' answers to 'definite' questions [24]. In terms of basic physicochemical property of combustion, answers were provided to tackle 'definite' questions such as,

- What is the flame speed change of bio-syngas combustion when ratio of H_2:CO concentrations varies from 1.0 to 1.1? Or, more specifically, for a parametric study, what are the flame speeds of bio-syngas combustion when the ratio of H_2:CO = 1.0 and 1.1 or other specific values?

Questions in a 'set of definite events' can be answered if in-depth knowledge of bio-syngas combustion is obtained either through experiments or numerical simulations, while questions in a 'set of probabilistic events' are hard to answer. In practical use of bio-syngas, probabilistic answers are needed to tackle probabilistic questions such as,

- What is the likelihood of flame speed change of bio-syngas combustion when ratio of H_2:CO concentrations varies from 1.0 to 1.1 are equally likely? Or, in a more specific term,
- If there is no evidence of whether in bio-syngas, ratio of H_2:CO concentration equals 1.0 is more likely than 1.1 or not (due to random variation of fuel composition), will the likelihood of obtaining high flame speed be higher or low flame speed be higher?

Probabilistic answers are of practical meanings to guide the use of bio-syngas as customers seek answers to confidence levels of using bio-syngas or risk assessments [25].

To quantify the role of fuel variability in bio-syngas combustion and provide confidence levels on its use, uncertainty quantification (UQ) methods [26] based on 'Sobol' decomposition is desired in place of conventional local uncertainty analysis/variance propagation method [27]. The latter method is only accurate when uncertainties of input parameters are small, and when linearity and normality assumptions hold. While for non-linear combustion problems involving high uncertainties in bio-syngas composition, the former method is more effective, and provides quantified confidence levels on using bio-syngas. Although 'screening' technique such as Morris method [28] can also identify important compositions, it only provides qualitative means of important measures to bio-syngas combustion performances, and is hence not preferred. In other words, UQ method analyses the whole variance range of input uncertainty (fuel composition variation) and provides quantified likelihood of the whole variance range of output uncertainty (combustion performances).

Moreover, UQ method not only quantifies the uncertainties in combustion performances propagated from uncertain variations of bio-syngas fuel composition, but also enables in-depth analysis of the influence of fuel variation on variation of combustion performances via global sensitivity analysis techniques. Such global analysis helps to identify major contribution sources (variations in fuel composition) to variation of combustion performances such as laminar flame speed, adiabatic flame temperature *etc.* Reducing variation of identified major sources of uncertainty depresses combustion uncertainties and improves confidence levels of using bio-syngas. With such information retrieved from global sensitivity analysis, guidance can be provided to the upstream gasification processes for targeted uncertainty reduction.

Recently, Wang and Sheen [29] reviewed uncertainty quantification, propagation, and minimization techniques. It was concluded that most of current UQ works have so far only focused on forward uncertainty propagation, where the uncertainty in the rate parameters of combustion kinetic models is prescribed. Indeed, Phenix et al. [30] studied supercritical water hydrogen oxidation mechanism using Monte-Carlo method and a so-called deterministic equivalent modelling method to determine the effects of uncertainties in reaction rate constants and species thermochemistry. The latter method is used to determine polynomial chaos expansion coefficients which are necessary for polynomial chaos expansion (PCE) based global sensitivity analysis. The standard-state heat of formation of HO_2 radical and forward rate constant for H_2O_2 dissociation are identified as the largest contributors to uncertainty in predicted H_2 and O_2 species concentrations. Skodje et al. [31] and Klippenstein et al. [32] used 'screening' based global sensitivity analysis to improve the chemical mechanism of combusting methanol, and found that $CH_3OH + HO_2$ and $CH_3OH + O_2$ reactions were the most important steps in setting the ignition delay time. To enable higher dimensional analysis ("dimension" refers to the number of variables in stochastic space) involving 176 uncertain parameters in rate constants and thermodynamic data, Ziehn and Tomlin [33] used high dimensional model representation (HDMR) based global sensitivity method to study sulphur chemistry in a premixed methane flame. Results demonstrated the effectiveness of HDMR for complex chemical mechanism analysis, and it was concluded that for certain cases, combining HDMR and screening method is more efficient than HDMR alone. Other studies such as auto-ignition of H_2/O_2 mixtures [34] or extinction limits of hydrogen/oxygen/nitrogen non-premixed flames [35] also used HDMR to analyse effects of uncertainties in rate constants or thermodynamic data due to the comprehensive reactions involved.

It is noticed that UQ based global sensitivity analyses have been effectively applied to examine uncertainties in thermodynamic and kinetic data of chemical kinetic models in order to improve combustion predictabilities or minimize uncertainties, while limited attentions were given to the role of uncertain variation in fuel constituent and challenge remains in understanding the fuel variability effect of such fuel mixtures.

The current study aims at tackling this challenge by investigating fuel variability effect on bio-syngas combustion performances via UQ based global sensitivity analysis and thus to provide guidance to effective use of bio-syngas by quantifying the contributions of important compositions. This paper is organised as follows. Section 2 introduces the methodology employed in the current study such as basics of PCEs and 'Sobol' indices accompanied with some assumptions made for the likelihood of variations in bio-syngas fuel composition. Section 3 presents the quantified combustion performances, *i.e.* adiabatic flame temperature and laminar flame speed, with respect to uncertain variations in fuel compositions. Parametric studies of sensitivity of