Applied Energy 114 (2014) 724–734

Contents lists available at SciVerse ScienceDirect

Applied Energy

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

Multi-zone modeling and simulation of syngas combustion under laminar conditions

Eliseu Monteiro [a], Abel Rouboa [a,b,*], Marc Bellenoue [c], Bastien Boust [c], Julien Sotton [c]

[a] CITAB, University of Trás-os-Montes and Alto Douro, Vila Real, Portugal
[b] IDMEC-FEUP, MEAM University of Pennsylvania, Philadelphia, USA
[c] Institute PPRIME, CNRS–ENSMA–University of Poitiers, Futuroscope, France

HIGHLIGHTS

- ▸ A multi-zone model is presented capable to predict the heat flux and the quenching distance of laminar syngas flames.
- ▸ Quenching distance of syngas–air mixtures decreases with increasing heat flux.
- ▸ This tool is essential for estimate the flame quenching properties where the measurement is not possible such as in engines.

ARTICLE INFO

Article history:
Received 11 March 2012
Received in revised form 27 July 2012
Accepted 2 August 2012
Available online 18 September 2012

Keywords:
Syngas
Wall heat flux
Quenching distance

ABSTRACT

The use of laminar models has been generally accepted, as quench distances in engines and the distances obtained for laminar flame quench calculations could be well correlated. In this work a multi-zone model is presented in order to derive the quenching distance and heat flux in laminar syngas–air flames based on recent developments in the science of combustion. Three typical mixtures of H_2, CO, CH_4, CO_2 and N_2 have been considered as representative of the syngas coming from wood gasification, and its laminar combustion is made in a static spherical vessel. The model is validated for the methane–air case and then applied to syngas–air mixtures in order to estimate the heat flux to the walls and quenching distances. Two wall heat transfer models are implemented and compared. The classical Woschni model based on the hypotheses of forced convection and the Rivère model based on kinetic theory of gases. Conclusion could be drawn that the Rivère heat transfer model is capable to better reproduce the heat flux to the walls. Heat flux through the walls is higher for stoichiometric syngas–air mixtures which follows the same behavior of the pressure inside the combustion vessel. Quenching distance of syngas–air mixtures decreases with the heat flux increase, which is consistent with earlier studies. This model could be very useful in predicting the physical conditions of quenching especially for estimation of the quenching distance where the measurement is not possible such as in engines. However, the estimation given should be understood as an order of magnitude, because in turbulent conditions the flame–wall interaction results in lower Peclet numbers than in the laminar case.

1. Introduction

As a result of environment and other policy considerations, there is increasing world-wide interest in the use of biomass resources as feedstock for producing power, fuels and chemicals. The gasification of biomass allows the production of a synthesis gas or “syngas”, consisting primarily of H_2, CO, CH_4, CO_2 and N_2 [1]. The specific composition depends upon the fuel source and the processing technique. These substantial variations in composition and heating value are among the largest barriers toward their usage. Elucidating the impact of this variability on combustor performance requires the knowledge of the fundamental combustion properties of these mixtures. Laminar flame speed is an important parameter of a combustible mixture as it contains fundamental information on reactivity, diffusivity, and exothermicity and have been subject of various studies in recent years [2–5].

Another important combustion parameter is the quenching of laminar, premixed flames at cold walls and is one of the classical problems in combustion science that has been studied extensively in the last 40 years [6–11]. In one of the first investigations, Daniel [6] estimated that up to 50% of the unburned hydrocarbons in the exhaust gas of internal combustion engines may originate from the quench layer on the cold wall. Information on quenching distances is also important since elevated temperatures near the walls of a

---

[*] Corresponding author at: MEAM Department, University of Pennsylvania, Philadelphia, USA.

E-mail address: rouboa@seas.upenn.edu (A. Rouboa).

0306-2619/$ - see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.apenergy.2012.08.027

Nomenclature

A	area of flame surface (m^2)
B	bore (m)
c_p	specific heat under constant pressure (J/kg K)
c_v	specific heat under constant volume (J/kg K)
D	diameter (m)
E	energy (J)
G	Gibbs free enthalpy (J)
g	specific Gibbs free enthalpy (J/kg)
h	heat transfer coefficient (W/m^2 K) or enthalpy (J/kg)
m	mass (kg)
M	molar mass (mol)
P	pressure (bar)
P_e	Peclet number
Q_w	wall heat flux (W/m^2)
Q_C	convective heat flux (W/m^2)
Q_r	radiative heat flux (W/m^2)
R	radius of the spherical vessel (m)
R_s	specific gas constant
R_u	universal gas constant = 8314 J/mol K
S	entropy (J/kg K)
S_u	laminar burning velocity (m/s)
S_{u0}	laminar burning velocity at reference conditions (m/s)
T	temperature (K)
t	time (s)
V	volume (m^3)
v	velocity (m/s)

Greek

α	absorption factor
δ_q	quenching distance (m)
Δt	time step (s)
ε	emissivity
ϕ	equivalence ratio
λ	thermal conductivity (W/m K)
μ	chemical potential (J/kg)
ρ	density (kg/m^3)
σ	Stefan–Boltzmann's constant ($J/m^2\ K^4$ s)
Y_{fuel}	fuel mass fraction
χ, ζ	constants

Subscripts

b	burned
F	flame
i	zone, species
in	inlet condition
out	outlet condition
t	total
u	unburned
w	wall
0, r	reference condition

Superscripts

α	laminar burning velocity correlation temperature exponent
β	laminar burning velocity correlation pressure exponent

combustion chamber degrade components, decreasing their lifespan [12]. Heat transfer has a significant impact on the efficiency of an engine, lowering the usable work when heat transfer rates to the chamber walls are high. Moreover, heat transfer affects, to a certain extent, the in-cylinder temperature distribution. Depending on the engine type, the temperature field affects the combustion process and the pollutants formation within the combustion chamber [13]. Finally, the effect of wall temperature on unburned hydrocarbon emissions from the quench layer has been the topic of some investigations [9,12,14].

Previous work [15] has shown that heat transfer to the walls is negligible, apart from the very final stages of combustion, which accounts for the lower than expected final pressure. This is detectable from the rate of pressure rise no longer increasing with time, leading to the rounding of the pressure record at maximum pressure and a change in the slope of the burning velocity when plotted against time. Indeed, the interest in flame–wall interaction is related to the problem of unburned hydrocarbons, as quenching distance determines the thickness of the unburned layer. Moreover, heat transfer models need accurate experimental data to perform near-wall calculations and to improve the evaluation of thermal losses. Therefore, a simplified model of flame–wall interaction is necessary to connect the main quenching parameters, such as quenching distance and heat flux [11]. The use of laminar models has been generally accepted, as quench distances in engines and the distances obtained for laminar flame quench calculations could be well correlated [7–9]. Moreover, studying flame–wall interaction in the laminar case is consistent with flow relaminarization that occurs in near-wall region [16]. An equation describing the behavior of single-wall flame quenching was derived from a simplified model of laminar flame–wall interaction by Boust et al. [11]. It allows evaluating quenching distance from wall heat flux and mixture properties; a significant advantage of this formula is the absence of any empirical coefficient and thus implemented in the proposed model.

These combustion processes have been modeled with zero-dimensional, multi-zone or multi-dimensional models [17]. The first two types are classified as thermodynamic models, where the equations constituting the basic structure of the model are based on conservation of mass and energy and are only dependent on time resulting in ordinary differential equations. Multidimensional models are also termed fluid dynamic models, where the governing equations are the Navier–Stokes equations in addition to conservation of mass and energy. Multi-zone models are distinguished from zero-dimensional models by the inclusion of certain geometrical parameters in the basic thermodynamic approach, such as the radius of the thin interface (the flame) separating burned from unburned gases, resulting in a ‘two-zone’ model and the sub-models of the mass burning rate (the laminar burning velocity) and wall heat transfer (the quenching distance). Every zone is initialized by different initial temperature and other needed parameters. Mass exchange and heat transfer between zones may be considered. A wide variety of multi-zone models has been published in the literature (see the excellent review of Yao et al. [18]). The main differences between the models can be categorized as follows: the number of zones, the kind of zones (e.g. adiabatic core zones, boundary layers, crevices and mass exchange zones), and the types of interaction that occur between zones (pressure–volume-work, heat transfer, mass exchange). Since the zones in the multi-zone models can represent crevices, boundary layers and core zones, the models are also referred to as being quasi-dimensional.

The choice of multi-zone or multi-dimensional model is largely determined by the application. If the objective is to evaluate a large range of conditions and perform parametric studies, a reasonable accuracy and fast computation is required. These conditions are