Applied Energy 162 (2016) 908–923

Contents lists available at ScienceDirect

Applied Energy

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

Application of an entrainment turbulent combustion model with validation based on the distribution of chemical species in an optical spark ignition engine

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HIGHLIGHTS

- 0D modeling of flame propagation and rates of heat release in an optical engine.
- Calibration based on in-cylinder pressure measurements.
- Validation of the entrainment concept using optical data.
- Stratification of chemical species confirmed through simulation and experiments.

ARTICLE INFO

Article history:
Received 27 July 2015
Received in revised form 28 September 2015
Accepted 20 October 2015

Keywords:
Spark ignition engine
Turbulent combustion
0D three zone model
Experimental validation
Flame visualization

ABSTRACT

Internal combustion engines are still the energy conversion units of choice in transport and distributed energy generation. Due to the fuel mix, spark ignition (SI) engines represent a viable solution that features improved fuel flexibility with respect to their compression ignition counterparts. Therefore, manufacturers are continuously trying to increase their performance and reduce emissions through experimental and numerical investigations. A growing trend in engine improvement is the application of simulations on a wider scale in order to contain development costs. Combustion is the most complex part of the working cycle and for SI power units, modeling flame propagation represents an essential feature of predictive numerical investigations. Within this context, the present study was aimed at better understanding the mass transfer between unburned and reacting gas, as well as characteristic reaction time scales within the reaction zone. A 0D model with three zones was applied for different engine speed, load, air-fuel ratio and spark timing settings, chosen as representative for mid-road load automotive use. Combined in-cylinder pressure measurements and flame imaging were used for validating the essential concept of fresh charge entrainment and burn-up process. One major conclusion of the work was that there is a definite stratification of chemical species within the burned-reacting gas that can be well captured by the entrainment model. The fact that the calibration coefficients require different values for accurate prediction of the pressure traces during flame propagation, emphasizes the complexity of the combustion process, as well as the limitations of considering flames as laminar even at local scale. The study also identified the scale at which mass transfer takes place as an essential factor for correct turbulent combustion modeling.

1. Introduction

Extensive efforts into the development of internal combustion engines are continuously undertaken by manufacturers and researchers, in order to ensure high energy conversion efficiency, reduced emissions, as well as increased degree of fuel flexibility [1,2]. An ongoing trend in engine research is the use of numerical simulations on an ever wider scale for reducing costs associated with experimental trials. For spark ignition (SI) power units, the most difficult task is to model turbulent flame front propagation, given the complexity of local mass transfer and chemical kinetics. Another phenomenon that is being intensely studied is the occurrence of abnormal combustion due to autoignition of the end gas before it has been reached by the normally propagating flame front [3]. This has become even more important as there is a generalized

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http://dx.doi.org/10.1016/j.apenergy.2015.10.136
0306-2619/

Nomenclature

A	area (m^2)
C	calibration coefficient (–); specific heat (J/kmol K^{-1})
h	specific enthalpy (J/kg)
l	characteristic length (m)
L	lift (m)
m	mass (kg)
M	molecular weight (kg/kmol)
Nu	Nusselt number (–)
p	pressure (Pa)
Pr	Prandtl number (–)
Q	heat (J)
Re	Reynolds number (–)
S	flame speed (m/s)
T	temperature (K)
u	entrainment speed (m/s)
U	internal energy (J)
V	volume (m^3)
x	mass fraction (–)
y	volume/molecular fraction (–)
η	efficiency (–)
λ	relative air-fuel ratio (–)
μ	parametric mass (kg)
ρ	gas density (kg/m^3)
τ	characteristic time (s)

Abbreviations

AFR	air-fuel ratio
ASOS	after start of spark
ICCD	intensified charged coupled device
CMOS	complementary metal-oxide semiconductor
COV	coefficient of variation
DI	direct injection
EVC/O	exhaust valves closure/opening
IVC/O	intake valves closure/opening
LHV	lower heating value
RMSE	root mean square error
SI	spark ignition
TDC	top dead center, with a- for after b- for before
WOT	wide open throttle

Subscripts

0	reference condition
b	burned
f	flame
ht	heat transfer
i	intake
iv	intake valve
l	length
L	laminar
p	piston/constant pressure
r	residual gas
st	stoichiometric
T	turbulent
u	velocity/unburned
v	volumetric
w	walls

trend of applying extreme boosting and downsizing for further improving fuel economy [4]. Low speed pre-ignitions have been designated as 'super-' or 'mega-knock' [5] and were found to be correlated to mixture stratification, local turbulence scale and temperature gradients [6].

Given the inherent complexity of turbulent combustion modeling, only 3D CFD codes can ensure the required detail for correct prediction of local transport phenomena. Nonetheless, 0D modeling can ensure a good compromise between accuracy and computational efforts [7]; also, the data obtained from the 0D simulations represent a good starting point for the more complex CFD investigations that can significantly reduce overall run-time [8]. With the introduction of stochastic sub-models, 0D codes can even predict cycle-to-cycle variations determined by the main parameters of influence [9]. For these reasons, the development of turbulent combustion models is continuously sought after, so as to improve predictive capabilities in a wide range of operating conditions. The basic approach of relating flame speed to turbulence intensity in the unburned zone is generally preferred, due to difficulties of applying direct numerical simulations in practical combustion systems [10]. In SI engines, three assumptions are usually employed when applying 0D/3D simulations. The first one is to directly relate the flame propagation speed to turbulence intensity and laminar flame speed [11], an approach that was found to give good results with different fuel types without requiring re-calibration [12]. Another method is to consider flame propagation as an essentially laminar process and that the increase in fresh charge oxidation rates is the effect of flame front wrinkling [13]. The actual increase in flame front surface (and therefore the rate at which unburned charge is consumed) can be defined by the use of fractals theory, that correlates the shape of the surface to the scales of turbulence during combustion [14,15]. The third approach is to apply an 'entrainment' equation, for which there is a reaction zone behind the flame front (with ongoing fuel oxidation), in-between the unburned and burned gas, thus resulting in a three zone model [16]. There are several variations of these basic approaches, with different ways of defining the flame front as well as mass transfer, and each one has specific challenges and advantages when applied for combustion simulation in SI engines [17].

No definite confirmation of one model or the other was obtained through measurements on a wide range of operating conditions. As an example, in some cases flame distortion and wrinkling seemed to have the opposite effect than that predicted by the second model [18] (i.e. the approach that considers the flame as basically laminar but with an increased surface), especially in the initial stages of combustion [19]. Another issue is that all three models rely on the value of laminar flame speed to account for fuel effects. For fuels that feature properties close to those of gasoline, this was found to be of relatively reduced importance with regard to accuracy if other effects such as in-cylinder evaporation are taken into account [20]. For other energy sources, such as hydrogen, this was found to be essential [21] and especially in extreme conditions with high exhaust gas recirculation rates [22].

One issue related to combustion modeling is that validation is carried out based on measurements of different thermodynamic parameters (e.g. for SI engines recording in-cylinder pressure is an established procedure [23,24]). Investigations based on the evaluation of gas density can be used for identifying islands of unburned regions behind the flame front and their size at different levels of turbulence [16]. Different chemical species (e.g. the OH radical is consolidated as a marker for oxidation reactions [25,26]) are used for validating chemical kinetic models that are