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Large-eddy simulation of flame-turbulence interaction in a spark ignition engine fueled with methane/hydrogen/carbon dioxide

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ABSTRACT

A three dimensional large-eddy simulation of in-cylinder charge and combustion process of a spark ignition engine was conducted. Partially stirred reactor combustion model and Arc and kernel tracking ignition model were implemented and applied to capture in-cylinder ignition and turbulent combustion. Interaction between flame and in-cylinder background turbulence for different mixtures of methane, hydrogen and carbon dioxide were studied. When a spark ignition engine is fueled with methane and carbon dioxide, its found that gas heating effect plays a dominant role in flame-induced turbulence. Increase of volume fraction of carbon dioxide has little effect on turbulent flame speed in each combustion phase defined by mean combustion progress variable, but it weakens gas heating effect owing to reduction in burnt temperature. Flame-induced turbulence produces small-scale vortices with high vorticity within gas preheating zone. When engine is fueled with methane, hydrogen and carbon dioxide, large volume fraction of hydrogen leads to high turbulent flame speed, which plays a dominant role in flame-induced turbulence. If volume fraction of hydrogen is small, flame-induced turbulence mainly is determined by gas heating effect due to large volume fraction of carbon dioxide. Flame-induced turbulence produces many vortex-pairs, which are the major sources of wrinkles of flame front. Rotation direction of vortex-pair determines whether the flame front bulges towards unburnt area or burnt area. Level of vorticity value and space size of vortex-pair affect sizes of wrinkles on the flame front.

1. Introduction

In light of today's shortage of petroleum based fuels and public concern regarding air pollution from combustion of fossil fuels, modern internal combustion engines are developed to utilize more alternative fuels with high efficiency and low emissions. Then the wide availability of gas fuels has led to lots of concerns and researches on gas fuels applications in internal combustion engines. The natural gas has been known as the high quality gaseous fuel. At the same time, several gaseous fuels such as biogas are becoming the research focus of new alternative energy fuels. The biogas is composed by 40–60% methane, 40–60% carbon dioxide. The advantage of biogas is that it can be produced close to the consumption points and hence is ideal for decentralized power generation in remote rural areas.

In the early stage, fundamental studies about premixed and partial premixed combustion of methane were conducted. The turbulent flame propagation regimes of methane–air mixtures have been identified [1], in which subsonic slow regime occurs in SI engines. A thermodynamic model was established to measure laminar burning velocity of methane–air-diluent mixtures in relative low pressure and temperature where carbon dioxide and nitrogen were used as diluents [2]. Then turbulent burning velocities of methane/air flame were measured with a range of high pressures and temperatures using Bunsen flame and OH-PLIF techniques [3]. An experiment on turbulent Bunsen flame was conducted to study turbulent Reynolds number and eddy scales affected by pressure variations [4]. The effect of turbulent parameters such as eddy scales on flame front was detailed analysed. In summary, combustion properties and influence of thermal conditions and transport coefficients were detailed researched. Then scholars managed to apply natural gas in SI engines and found that lean burn becomes an efficient and applicable way when engine is fueled with natural gas. In order to meet future stringent emission regulations, stoichiometric natural gas engines equipped with three way catalyst could be a good choice [5]. On the other hand, biogas was used as fuel in IC engines [6], and dual-fuel containing biogas and diesel seemed to be preferable due to biogas' reduced fuel cost [7]. However, cycle-to-cycle variation becomes a urgent problem because of long combustion duration when natural gas or biogas is burnt in SI engine.

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Nomenclature

$\bar{\dot{w}}_i$	mean chemical reaction rate of ith step
$\bar{\rho}$	filtered density
$\bar{p}$	filtered pressure
$\bar{\mathbf{D}}$	the large-scale strain rate tensor
$\boldsymbol{\tau}$	sub-grid scale stress tensor
$\boldsymbol{I}$	unit tensor
Δ	spatial filtered scale
δ_L	laminar flame thickness
γ	motion diffusivity of node
$\bar{\mathbf{S}}$	strain rate tensor
K	sub-grid turbulent kinetic energy
u_c	cell center velocity
Y_i	mass fraction of specie i
v	laminar kinematic viscosity
v_{sgs}	SGS eddy viscosity
v_l	molecular viscosity
v_t	turbulent viscosity
Σ	flame wrinkling
τ_c	chemical time scale
τ_d	viscous diffusion time
τ_{mix}	micro-mixing time scale
$\tilde{\mathbf{u}}$	Favre filtered velocity vector
ε	dissipation rate of TKE
Ξ	sub-grid flame surface wrinkling factor
ATDC	after top dead center
b	combustion progress variable
BTDC	before top dead center
C_ε	model coefficient
C_k	model coefficient
CA	crank angle
CCV	cycle-to-cycle variation
D_F	fractal dimension of the turbulent field
DNS	direct numerical simulation
EVC	exhaust valve closing
EVO	exhaust valve opening
IC	internal combustion
IVC	intake valve closing
IVO	intake valve opening
l_0	initial length scale of eddy
l_{sgs}	sub-grid eddy length scale
l_{spk}	gap of spark plug
LES	large-eddy simulation
RANS	Reynolds average Navier–Stokes
Re	Reynolds number
SI	spark ignition
TDC	top dead center
x_{spk}	position of spark plug

Essentially, cycle-to-cycle variation is a traditional obstacle in IC engines. For the sake of improvement in engine operation, a large number of studies began to focus on identifying causes of CCV. It was proposed that variations of fuel, amount of EGR and air contribute to CCV only by 5–10%, and the rest is mainly caused by turbulence in engines [8]. Experiments showed that if the fuel and air are well mixed and the engine load is high, the dominant cause of CCV in the early combustion is the flow situation in the vicinity of the spark plug, but when port injection is introduced, dramatically increased CCV could be explained by the fluctuating fuel concentration [9]. They also figured out that variations of temperature and EGR composition have little effect on CCV. Recently, advance in computer leads to available large numerical simulations to explore CCV from a mechanism angle. It's proposed that in engines composition variations scarcely alter turbulent flow structure [10]. Some studies have been done on large-scale turbulence in engines and it was found that variations of combustion rate correlates with shear strain rate, vorticity and velocity [11]. Variations of flow in the vicinity of spark plug and composition inhomogeneity are crucial factors affecting formation of initial flame kernel and subsequent flame propagation, which finally has a great effect on CCV [12]. Combining LES and advanced G equation combustion model to numerically analyze CCV of port injection SI engine, the result showed that early formation and growth of flame kernel is related to flow turbulent kinetic energy while cyclic variation of laminar flame speed has little effect on CCV [13]. Multi-cycle simulations were conducted and the conclusion was that variation of flow velocity around spark plug is the main factor of CCV [14].

Now that CCV strongly depend on formation and development of initial flame kernel, thus studies about flame kernel have been conducted and some valuable conclusions are drawn. For flame kernel in premixed gases, its believed that the amount of input electrical energy is important in the location of flame, but the geometry of the spark electrode does not affect flame speed and location of flame, and flame needs a certain amount of time to become self-sustained [15]. It is extended that turbulence plays a crucial role in formation of stable flame kernel rather than spark plug configuration. Reddy et al. [16] have studied on ignition kernel development relevant to lean-burn-gas engines and concluded that as long as available ignition energy is greater than a minimum, the duration in which a stable speed is reached is relevant to kernel temperature. They [17] also use direct numerical simulation (DNS) method to study influence of flow velocity and length scales on development of formed flame kernel at elevated pressures and temperatures relevant to engines. A non-dimensional number defined as ratio of turbulence length scale and spark plug gap and velocity fluctuation are applied to divide interaction between flame and turbulence into three regimes, which means that difference in length scales and turbulence intensities leads to different flame kernel shape. Furthermore, interaction between flame and turbulence will wrinkle flame front. Cyclic variation of flame front area will affect CCV [18]. Subsequent studies indicated that when engine operates at high rotation speed, wrinkle of flame front and cyclic variation of flame front area contributes to CCV about 15% [19]. Now studies relevant to formation of flame kernel or its interaction with turbulence are carried out a lot as mentioned above, and inhomogeneity's effect also studied in great detail [20]. Some other studies about piston engine are mainly focused on knock predication [21] and new combustion mode like HCCI [22]. Studies of flame-turbulence interaction in latter stage of flame propagation in gas fueled engines, are rarely involved. It's necessary to study how flame interacts with in-cylinder background turbulence, which is also important factor that influences CCV in gas fueled engines. So the aim of authors is to establish a three dimensional numerical simulation model based on LES method and study interaction between turbulence and flame front in a SI engines fueled with $CH_4/H_2/CO_2$, thus to find effect of fuel composition on flame-turbulence interaction. The different combinations of methane and carbon dioxide simulate various kinds of biogas. In this work, composition inhomogeneity factor is excluded by perfectly mixing methane and air in intake port instead of port injection.