

CFD Contextual Modelling of Biogas Combustion in Internal Combustion Engine: A Review

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Abstract: The perpetual use of petroleum products as fossil fuel nowadays is the primary cause of many economical, ecological and environmental problems. The exhaust emissions from fossil-fuelled engines world over are a major cause of hazardous emissions such as NO_x (oxides of nitrogen), CO (Carbon monoxide), HC (Hydro Carbons) and PM (Particulate Matter). Furthermore high temperature combustion in fossil-fuelled IC engines has been identified as the major contributor of greenhouse gases characterised by high pollution emissions. Hence this review paper focuses on findings from contemporary renewable energy researchers based on attempting to substitute fossil-fuelled IC engines with biogas fuelled ones. Recent studies have been focusing on combustion modelling and technology that would lead to the improvement in biogas combustion efficiency. Confirmation from literature indicates that biogas usage as an engine fuel has the greatest potential of substituting the environmental unfriendly fuel derived from petroleum products due to its very low CO₂ emissions. CFD simulations based on biogas combustion have further proved that high energetic contents of biogas similar to that of natural gas can be combusted for the generation of mechanical energy. The SA automotive industry is growing fast but still based on fossil-fuelled IC engines. Hence, the findings from literature suggest the need to develop CFD modelling of biogas combustion in internal combustion engine in the context of SA automotive industry.

Keywords: *Computational Fluid Dynamics, Compression Ignition, internal Combustion, Navier Stokes Equations, Spark Ignition, Combustion Modelling.*

1. INTRODUCTION

Energy is universally recognized as a prime agent of economic development [1]. Contemporary energy researchers have already verified the existence of a relationship between energy availability and economic activity [2]. Rapid growth in world economies together with associated exponential increase in population has led to an abrupt increase in energy demand [3]. About 80% of overall energy demand is mainly derived from fossil fuel [4].

In the recent years fossil fuel prices have been on the rise due to limited supply and deposits especially of crude oil as well as significant increase in demand of petroleum fuels [5]. The reality of risks associated with environmental degradation and climate change due to petroleum fuel usage are now more apparent [2]. Carbon monoxide, sulphur dioxide, nitrogen oxides and particles are undesirable emissions associated with burning fossil fuels. These compounds are toxic, contribute to acid rain and smog and can ultimately cause respiratory problems. The automotive industry is world's primary consumer of energy extracted from fossil fuels [6]. The current rate of energy consumption from fossil fuel sources means that all reservoirs will be depleted by 2042 [7]. Furthermore high temperature combustion of fossil fuels has been identified as the major contributor of greenhouse gases due to its high pollution emissions [8]. Currently, a fossil fuel derivative like diesel (a mixture of hydrocarbons with C₁₅ - C₁₈ carbon atoms and an approximate calorific value of about 11,000 kcal/kg) is used as fuel in compression ignition engines. However, the perpetual use of petroleum products like diesel as fossil fuel nowadays is the primary cause of many economical, ecological and environmental problems. For instance, the exhaust emissions from the diesel engines world over are a major cause of respiratory problems and, heavy pollutions with hazardous emissions such as (oxides of nitrogen (NO_x), Carbon monoxide (CO), Hydro Carbon (HC) and Particulate Matter (PM) [9].

The primary reason for this pollution is due to the heterogeneous mixture of air and diesel in the combustion chamber. This fuel will be exhausted soon because of its excessive usages and non-renewable nature. The most critical issue in the present is the replacement of fossil fuels with renewable sources. Renewable energy resources are potentially among the most effective and efficient solutions to non-renewable sources such as fossil fuel. Suggesting that the use of alternative energy source in internal combustion (IC) engines will have greater impact on energy generation and consumption [10]. It is against such a catastrophic background that an alternative automotive fuel resource is required to meet the requirements of the current environment to reduce hazardous emissions without compromising CI engine efficiency. Hence, biogas is a better alternative fuel, which can be used to circumvent the above crisis [11]. Furthermore, reducing consumption of oil-derived energy products will greatly minimize greenhouse gas emissions [12]. A renewable energy source like biogas is what the future holds even for the automotive industry. It is therefore imperative to simulate and analyse the fundamental impacts of firing biogas in an IC engine using CFD analysis methods. This will help to accurately predict the physical conditions required before engineers can modify the engine into accepting biogas as fuel.

2. COMBUSTION ENGINE SYSTEMS

There are two main types of combustion engines namely internal combustion engine (IC) and external combustion (EC) engines [11]. The compression ignition (CI) engine and Spark ignition (SI) engine exist as the two types of IC engines in the auto-industry. The combustion process in a SI and CI engine can easily be described through use of Wiebe equation shown [13].

$$x_b = 1 - \exp \left[-a \left(\frac{\theta - \theta_0}{\Delta t} \right)^{m+1} \right] \quad (1)$$

Where θ = crank angle, θ_0 = the position of the crankshaft angle at which the spark was ignited, Δt = the total combustion duration, a and m are adjustable parameters with a representing the maximum fraction of energy released/burned mass, ($x_b = 0$ to $x_b = 1$). However in mechanical engineering, the CI engine is preferred to SI due to its high thermal efficiency, low fuel consumption and very low emissions of uncombusted hydrocarbons [14].

In an IC engine ignition the combustion process is generally characterised by spark timing as well as duration and completeness of combustion [11].

2.1 Internal Combustion Engine

Internal combustion (IC) engine is widely used for fuel combustion particularly in the automotive industry [15]. It is important to improve the engine efficiency through reduction in fuel consumption, hazardous emissions, noise pollution and the negative effect these leaves on the environment [16].

The IC engine exists in many different types and sizes but can all be categorised as two-stroke cycle or four stroke cycle. The following are examples of internal combustion engines:

- Compression ignition (CI) also called single fuel non-premixed compression ignition engine. (SFNPCI)
- Spark ignition (SI) also called the single fuel premixed spark ignition engine (SFPSI)
- Homogenous charge compression ignition (HCCI)
- Reactivity controlled compression ignition (RCCI) also referred to as the dual fuel premixed compression ignition engine. (DFPCI)
- Variable compression ratio (VCR)
- Opposed piston internal combustion engine (OPICE)

The IC engine can either be run by Otto or the Diesel principle. For Otto IC engines, a spark from a spark plug [17] ignites the pre-mixed air-fuel mixture. For the Diesel principle, the air is compressed beforehand in the cylinder and the incoming fuel spray is ignited by the high pressure and temperature [18]. In spark-ignited (SI/Otto) engine, the four-stroke cycle according to Chiodi [19], starts with the piston positioned in top dead centre (TDC) and as the piston travels down towards bottom dead centre (BDC) the intake valve opens, letting the fresh charge of air-fuel mixture to enter the cylinder during the *intake stroke*, as shown in Figure 1a. With the piston at BDC the intake valve closes and as the piston travels towards TDC again the fresh charge is compressed during the *compression stroke*, see Figure 1b. As the piston reaches TDC the compressed air-fuel mixture is ignited by the spark plug and the chemical energy of the fuel is converted to heat during combustion. This increases the cylinder gas temperature and pressure, thereby adding work to the crankshaft during the power stroke or *expansion stroke*, see Figure 1c. When the piston reaches BDC again the exhaust valve opens and as the piston travels towards TDC the exhaust gas is pushed out from the cylinder during the *exhaust stroke*, see Figure 1d. When the piston has reached TDC the cycle is restarted again. In one power cycle the crankshaft has done two full revolutions (720 crank angle degrees or CAD) and the piston has travelled up and down the cylinder four times, therefore the name four stroke cycles.

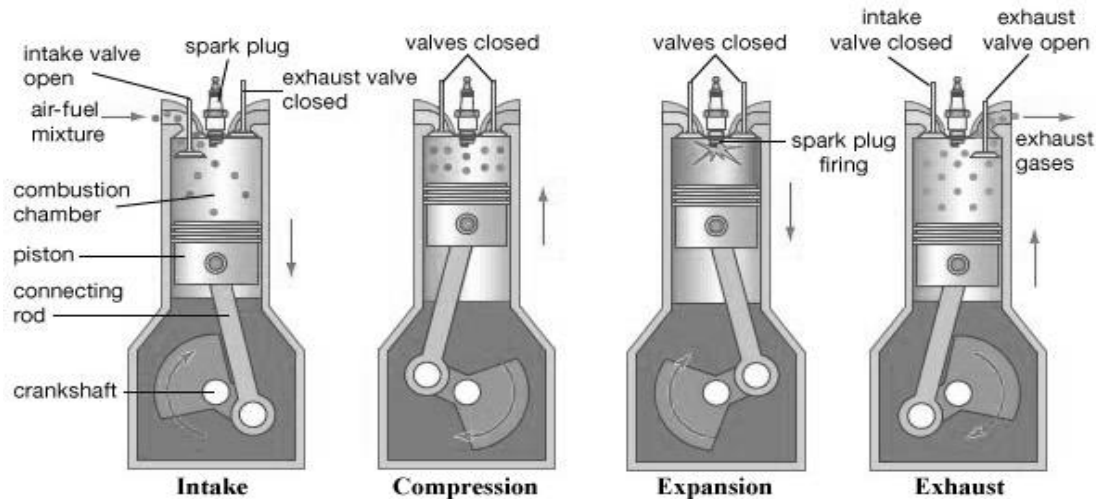


Figure 1: The four stroke cycle (adapted from Semin, 2008)

3. POTENTIAL OF BIOGAS AS FUEL FOR IC ENGINES

Biogas is a renewable energy fuel derived from anaerobic digestion of organic matter such as municipal and agricultural wastes [13]. Biogas is mainly composed of a mixture of methane (CH_4) and carbon dioxide (CO_2) [12]. The heating value of biogas depends primarily on its CH_4 content [19]. The methane composition of biogas produced in most anaerobic digesters ranges between 40% -75% [20]. Under standard conditions of temperature and pressure, methane has a density of approximately 0.75kg/m^3 [15]. Adding carbon dioxide that is slightly heavier, the biogas density reaches about 1.15kg/m^3 [12]. Pure methane has an upper calorific value of 39.8MJ/m^3 , which corresponds to 11.06Kwh/m^3 [19]. The quality of biogas from a biogas digester plant (BDP) varies with period of digestion (adapted from Reddy & Reddy, 2014). Biogas of higher quality burns with a blue flame in the presence of excess oxygen (O_2) [21].

The use of biogas as an engine fuel is advantageous due to its low CO_2 emissions [13]. Biogas has the capability of lowering the ignition limit and can increase the power output by augmenting the energy density at lean mixtures hence, increasing the biogas-to-carbon ratio [22]. Biogas cannot be used directly in a compression ignition engine because of its high auto ignition temperature [23]. Huang & Crookes [14] recommended pilot ignition techniques in which diesel engines is fitted with spark plugs or a use of small amount of diesel fuel to ignite the biogas.

The combustion of a mixture of biogas and air produces low gas temperature inside the combustor compared to natural gas (Mihic, 2004). The biogas combustion temperature depends on the carbon dioxide to methane ratio (CO_2/CH_4) (Razbani, et al., 2011). The biogas temperature decrease by about 37% for every 22% increase in CO_2/CH_4 ratio.

Huang & Crookes [14] observed that the NO_x emissions inside a combustor decreases when diesel or gasoline fuel is replaced with biogas due to lower heating value. Noting that thermal NO_x emission is a function of gas temperature, thus high gas temperature produces high NO_x (mainly NO) emissions [24]. The presence of non-combustible constituents in the biogas such as carbon dioxides and nitrogen also reduces the temperature of the flame and consequently the NO mass fractions [15].

The NO_x emissions at the exit point of the combustor decreases with increase in biogas CO_2/CH_4 ratio but the emissions of CO_2 at the exit of the combustor increase with an increase of CO_2 fractions in the biogas fuels (higher CO_2 input) [22]. The presence of non-reactive gas (CO_2) with methane cools down the reaction by absorbing energy from the combustion and modifies the reaction zone by reducing flame burning rate and velocity [15]. The emissions from biogas combustion vary with the composition of biogas. The higher CO_2 percentage in the biogas fuel, the lower the NO_x emissions and the higher the CO_2 emissions at the exit point of the combustor. The CO emissions also decrease by increasing the CO_2/CH_4 ratio of the biogas fuel [24].

4. COMPUTATIONAL FLUID DYNAMICS

Many computational tools aid in the design and development of IC chambers and analysis of combustion process with the aim of improving combustion efficiency [25]. Computational fluid dynamics (CFD) is a computational tool that can be used in calculating combustion dependent parameters as well as combustion process. CFD uses a numerical method in solving a set of non-linear partial differential equations to predict fluid flow. The complex engineering problems solved using CFD approaches involve turbulence [11], hot spots analysis, compression ratios, ignition limits, ignition timing [26], emission pollutants and performance of combustors. [15].

The fundamental governing equations of computational fluid dynamics include continuity, momentum and energy equations [17]. These equations are focused on three basic parameters:

- a) Mass is conserved. (continuity equation)
- b) $F_{\text{net}} = ma$ (Newton's second law), momentum is conserved
- c) Energy is conserved.

The Navier-Stokes (NS) equations are a set of non-linear partial differential equations used to describe the flow of a fluid whose stress depends linearly on velocity gradients and pressures [17]. The NS equation ignores the fact that the fluid is made up of discrete molecules. To quantify the transition between laminar and turbulent flows then Reynolds number is preferably used [27]. The conservation laws are a statement of the fact that the rate of change of mass, momentum, or energy in a certain volume is equal to the rate at which it enters the borders of the volume plus the rate at which it is created inside [3].

4.1 COMPUTATIONAL MODELLING

The main concept of CFD is the discretized solution of a set of partial differential equations commonly known as the Navier-Stokes equations [21]. These equations are discretized in time, by solving the equations in small time steps, and in space by dividing the domain in a large number of small computational cells or control volumes (CV) [15]. The space discretized solution domain is commonly referred to as the computational grid or mesh [28].

The method commonly used for space discretization is called the Finite Volume Method (FVM), and for a static mesh (no moving boundaries), it is based on the integral form of the conservation equation over a control volume fixed in space [18]. The simulation of a fluid dynamics in a combustion engine requires moving boundaries of the solution domain, because the structure of the flow field is very much dependent on the moving piston and valves [15]. When the mesh has moving boundaries the integral form of the conservation equation for a tensorial property ϕ defined per unit mass in an arbitrary moving volume V bounded by a closed surface S is given in equation 2.

$$\frac{d}{dt} \int_V \rho \phi dV + \oint_S dS \cdot \rho \phi (u - u_b) = - \oint_S dS \cdot \rho q_\phi + \int_V S_\phi dV \quad (2)$$

where ρ is the density, u is the fluid velocity, u_b is the boundary velocity and q_ϕ and S_ϕ are the surface and volume sources/sinks of ϕ respectively [19].

The CFD equations govern the flow of fluid [2]. The conservation form of CFD governing equations is obtained directly from a control volume that is fixed in space rather than moving with the fluid [17]. When the volume is fixed in space the concern is on i) the flux of mass into and out of volume. ii) momentum into and out of the volume. iii) energy into and out of the volume [12].

4.1.1 Governing Equations

The governing equations used for biogas combustion include equations of conservation of mass, momentum, energy, equations of the turbulent kinetic energy κ , and the dissipation rate of the turbulent kinetic energy the ε standard $\kappa - \varepsilon$ turbulence model), the mixture fraction equation (mixture fraction/PDF (probability density function)) model for non-premixed combustion modeling), and the equation of state. For steady turbulent non premixed combustion [29] the time averaged gas phase equations are given below.

THE CONTINUITY EQUATION

The continuity equation governs the conservation of mass, which means that the rate of change of mass in an arbitrary control volume must be equal to the total mass flow over the control volume boundaries:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0 \quad (3)$$

CONSERVATION OF MOMENTUM

The momentum equation governs the conservation of linear and angular momentum. According to Newton's second law, the rate of change of momentum on a fluid particle equals the sum of forces acting on that particle:

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = \rho g + \nabla \cdot \sigma \quad (4)$$

Where the two right hand terms denote the gravitational body force and viscous stress tensor respectively.

CONSERVATION OF ENERGY

This equation is based on the first law of thermodynamics which states that the rate of change of total energy of a fluid element (internal, kinetic, mechanical, chemical energy) must equal the net rate of heat and work flow over its boundaries [30]. However, an alternative formulation of the energy equation, used in the ANSYS FLUENT code, is the enthalpy equation:

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho u h) - \nabla \cdot [\alpha + \alpha_t] \nabla h = Q + \frac{Dp}{dt} \tag{5}$$

where ρ is the density, u is the fluid flow vector, g is the body force, σ is the stress tensor, h is the enthalpy, α is the thermal diffusivity for enthalpy, α_t is the turbulent thermal diffusivity, Q is the energy source term, and p is the fluid pressure.

MIXTURE FRACTION EQUATION

$$\frac{\partial (\overline{\rho f u_j})}{\partial x_j} = \frac{\partial \left[\left(\frac{\mu_t}{\sigma_t} \right) \frac{\partial \overline{f}}{\partial x_j} \right]}{\partial x_j} + S_m \tag{6}$$

The mixture fraction f is given by

$$f = \frac{(Z_k - Z_{k,O})}{(Z_{k,F} - Z_{k,O})} \tag{7}$$

Where Z_k is the element mass fraction of element k . Subscripts F and O denote fuel and oxidizer inlet stream values, respectively. S_m is the term source that includes the mixture of chemical species.

EQUATION OF STATE

Assuming that the biogas behaves ideally, then the equation for the temperature and the pressure can be given as

$$T = \frac{1}{R_0} \sum_i M_i \left[h_i(T) - \frac{\rho_i}{\rho} E(T) \right] \tag{8}$$

And

$$p = R_0 T \sum_i \frac{\rho_i}{M_i} \tag{9}$$

where M_i is the molar mass of species i and R_0 is the ideal gas constant

Thermodynamic relation between state variables is given by

$$e = e(T, p) \tag{10}$$

and for a calorically perfect gas this relation would be

$$e = c_v T \quad (11)$$

where c_v = specific heat at constant volume.

THE VELOCITY EQUATION

$$V = \sqrt{0.2gd \left(\frac{\rho w}{\rho b} \right)}, m \cdot s^{-1} \quad (12)$$

THE PRESSURE EQUATION

$$P = \rho wgh, N \cdot m^{-2} \quad (13)$$

THE REYNOLDS NUMBER

$$R_E = \frac{\rho bVD}{\mu_g}, \text{ dimensionless} \quad (14)$$

The NS equations are very difficult to solve. As the Reynolds number is increased, the scale of the interesting dynamics gets smaller so that most solutions of the full NS equations are done at Reynolds numbers of 1 to 10,000 for simple geometries.

COMPRESSION RATIO (C_R)

$$C_R = \frac{V_{BDC}}{V_{TDC}} \quad (15)$$

where V_{BDC} is the total volume of combustion chamber when piston is at the bottom of its stroke, V_{TDC} is the total volume of the combustion chamber when the piston is at the top of its stroke.

THERMAL EFFICIENCY (ξ_T)

$$\xi_T = 1 - \frac{1}{C_R^{k-1}} \quad (16)$$

Where k represents ratio of specific heat, a property of air.

4.2 Turbulence Modelling

The flow in the engine room is time dependent, unsteady, compressible and turbulent [28]. Turbulent flow is a flow that is irregular, random and chaotic [17]. It can be described as a state of continuous instability in the flow, where it is still possible to separate the fluctuations from the mean flow properties [21]. Turbulence is associated with eddies which affects the mean flow, where the range of the scales is very large, from the smallest turbulent eddies characterized by Kolmogorov microscales, to the flow features comparable with the size of the geometry. The largest eddies extract their energy from the mean flow [31]. These eddies transfer energy to smaller eddies in a cascade process. The large scale eddies have an orientation imposed by the mean

flow, but the smaller eddies will not “remember” their origin and orientation and will behave isotropic that is independent of direction. The scale of these eddies, referred to as Kolmogorov’s microscale, are small and dissipative forces prevails [19]. In this regime, the kinetic energy is destroyed by viscous forces, and viscosity and dissipation affect the length scales [18]. The cascade process, from the biggest to the smallest eddies, occurs over a wide length scale spectrum and a very fine mesh is needed to resolve the smallest Kolmogorov eddies.

4.2.1 Averaging methods for NS equation

A very fine resolution in time is also needed, since turbulent flow is always unsteady. The requirements on mesh resolution and time-step size for an exact solution of the flow, puts very high demands on computer resources, rendering it unsuitable for engineering applications [17]. This can be solved by simulating turbulent flow using statistical methods.

Using statistical or averaging methods, the local value of the variable can be separated into the mean and the fluctuation around the mean which then makes it possible to derive the equations for the mean properties themselves [19]. The averaging methods can appear in two versions, *Reynolds averaging* and *density-weighted Favre averaging*.

Most CFD packages (including ANSYS FLUENT) are to solve the Reynolds Averaged Navier Stokes (RANS) equations [18].

RANS equations govern the *mean* velocity $\bar{u}(y)$ and pressure but are primarily used to solve mean velocity only. If we formally average the NS equations and simplify for this geometry we arrive at the following

$$\frac{\partial \overline{u} \overline{v}}{\partial y} + \frac{1}{\rho} \frac{\partial \bar{p}}{\partial x} = \nu \frac{\partial^2 \bar{u}(y)}{\partial y^2} \quad (17)$$

Where $\overline{u} \overline{v}$ is known as the *Reynolds stress tensor*. Applying the averaging procedures to the NS equations will introduce the unknown term *Reynolds stress tensor*. This generates a NS system of equations with more unknowns, situation commonly referred to as the closure problem. To close the system, further modeling is necessary to solve the Reynolds stress tensor (Alias, 2008). A widely used method to handle the closure problem is the *Boussinesq approximation*, which states that the Reynold stresses are linked to mean rates of deformation by introducing a turbulent viscosity ν_t [19].

The turbulent viscosity ν_t can be evaluated through use of the $k - \varepsilon$ turbulence model.

4.2.2 The $k - \varepsilon$ Turbulence Model

This two-equation model makes use of two partial differential equations for the determination of the turbulent viscosity (Alias, 2008). k and ε are related to the primitive variables through

$$\tilde{k} = \frac{1}{2} \tilde{u}^2 \quad (18)$$

Where k is the turbulent kinetic energy

And

$$\tilde{\varepsilon} = \frac{\mu}{\rho} \overline{\nabla \vec{u}^T : \nabla \vec{u}} \quad (19)$$

Where ε is the turbulent dissipation rate and $\frac{\mu}{\rho} = \nu_L$ is the laminar viscosity.

The turbulent viscosity ν_t can then be calculated using the Prandtl-Kolmogorov equation [17] This equation expresses ν_t as a function of the turbulent kinetic energy k and its dissipation rate ε is given as

$$\nu_t = C_v \frac{\tilde{k}^2}{\tilde{\varepsilon}} \tag{20}$$

Where C_v is an empirically determined model constant ($C_v = 0.09$) while k and ε are obtained by the solution of their respective transport equations.

4.3 Combustion Modelling

The combustion model used for the simulations in this study is the $b - \Xi$ Weller combustion model because it is the standard combustion model incorporated in the ANSYS FLUENT CFD code [28]. This model is based on the evaluation of the dimensionless variable b that describes the species concentration of the combustion reactants in each computational cell [19]. The value of b ranges from 0 to 1. Where a value of 0 means that the combustion process is completed in the whole cell and a value of 1 means that no combustion process has taken place.

The transport equation to describe the evolution of b in time and space states:

$$\frac{\partial \bar{\rho} \tilde{b}}{\partial t} + \nabla \cdot \bar{\rho} \tilde{u} \tilde{b} - \nabla \cdot \Gamma_b \nabla \tilde{b} = - [\bar{\rho} \Xi + (\bar{\rho}_u - \bar{\rho}) \min(\Xi, \Xi_{eq})] S_u |\nabla \tilde{b}| \tag{21}$$

Where ρ is the density, ρ_u is the density in the unburnt mixture, u is the fluid flow vector,

$$\Gamma_b = \frac{\bar{\mu}_t}{\sigma_h} \tag{22}$$

Where μ_t is the turbulent viscosity, σ_h is the turbulent Prandtl coefficient, S_u is the laminar flame speed. The sign $\bar{\cdot}$ indicates the average and $\tilde{\cdot}$ indicates the Favre average based on the density (i.e. $\tilde{\mu} = \overline{\rho u} / \bar{\rho}$). The subscript eq signifies the equilibrium value which serves as an upper limit of Ξ . Lastly, Ξ is defined as the local flame wrinkling factor and it is defined as the ratio between the turbulent flame speed S_t and the laminar flame speed S_u :

$$\Xi = \frac{S_t}{S_u} \tag{23}$$

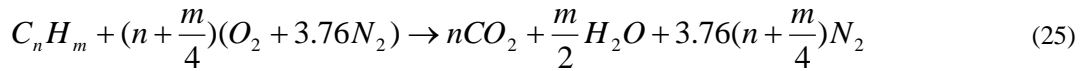
In solving for Ξ one can use a transport equation, which requires reproducing all the details of the flame structure or the transient response of the turbulent flame speed [12]. Under these conditions the Ξ transport equation need not be solved at all, instead a simple analytical (or algebraic) expression for Ξ can be used in the b equation.

Hence, the algebraic expression of Ξ is the given as:

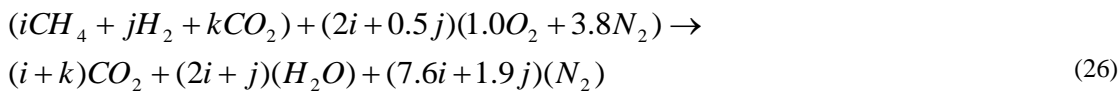
$$\Xi = \Xi_{eq} = 1 + A \left(\frac{u'}{S_u} \right) \quad (24)$$

where A is a free coefficient, u' is the turbulence intensity and S_u is the laminar flame speed.

The general hydrocarbon stoichiometric equation in a combustion process can be expressed as shown equation 25 [28].



For biogas stoichiometry the general form of combustion equation is given as



Where i , j , and k represent the mole fraction of CH_4 , hydrogen (H_2) and CO_2 respectively. The detailed study carried out on models used for internal combustion, spray, and auto-ignition to using CFD are presented below.

5. BIOGAS COMBUSTION SIMULATION STUDIES

The literature presented here shall predicate more on combustion modelling which have been studied, simulated and experimentally validated world over.

Porpatham [32] examined and modelled the effect of methane concentration on combustion in biogas fuelled SI engine. The observations from the study indicated that raising methane concentration in biogas led to the significant increase in SI engine performance and sudden reduction in total hydrocarbons (THC) emissions. Furthermore, the abrupt decrease in CO_2 concentration from biogas resulted in greater methane/ oxygen content in the charge leading to a faster combustion rate and tremendous power output at specific equivalence ratio. The simulated outcome of this study was validated and its results were found to be in agreement with experimental.

Another study reported that an increase in the concentration of CO_2 in biogas fuel led to a decrease in engine power output thus compromising engine performance. This also resulted in more production of pollutant compared to methane rich biogas. The efficiency of the IC was compromised with an increased fraction of CO_2 , which led to more consumption of biogas fuel for similar power output. Although the mole fraction of NO_x decreased significantly, the exhaust CO and THC concentration increased with increase in mole fraction of CO_2 [33].

Intensive studies on the Biogas-Diesel dual fuel combustion system was done by Shaik et al [34] using CFD analysis aided with ANSYS FLUENT Software package. In this study the benefits of biogas substitution in an IC engine in terms of combustion flame velocity (CFV) and probable formation of NO_x was simulated for five compression ratios. The κ - ϵ turbulence model was modified to aid in simulating turbulent kinetic energy (TKE) and turbulent dissipation rate (TDR) for the dual fuel system. The effect of compression ratio in ignition engine system in which biogas was premixed with air and diesel as primary fuel in this dual fuel set up was simulated.

Guessab et al [35] carried out a turbulent swirling flow analysis while applying a three dimensional RANS-RSM turbulence procedures for diffusion chamber, using biogas as fuels. The study was conducted using a can-type gas turbine combustor model. The flame was stabilised by gradually adding CO_2 at lean fuel/air equivalence ratios needed in the reduction of NO_x emissions. There was a significant change in aerodynamic and thermal properties when methane/natural gas was substituted with biogas. This was due to increase in fuel mass flow variations and lower heating value associated with biogas. This is because the two gaseous fuels differ in terms of their chemical composition. The results of the study were considered cost-effective as they significantly proved the possibilities of using methane or biogas in turbulent combustion systems.

In a study based on combustion of synthetic gases in an IC engine, Arroyo, [10] concluded that CO/CO_2 percentage is the major contributory factor of increased exhaust gas pollutants if compared with biogas and other related fuels. It was also observed in this study that the exhaust gas concentration of THC was relatively low due to the small-unburnt methane content. Although the presence of such chemical species like excess air and CO_2 provided mitigation for NO_x emissions. However greater mole fraction of H_2 in the synthetic gas led to an increased NO_x emissions being excreted by high combustion flame temperatures associated with the presence of H_2 .

Huang [36] studied a variable compression ratio (VCR) single cylinder SI engine fuelled with biogas. The simulation of the biogas operated VCR SI engine was achieved with different mixtures of domestic natural gas and CO₂. The content of CO₂ was gradually increased from 0% to 40% in order to replicate a biogas fuel. A range of air/fuel ratios were also studied from the lean to the rich operating limit at various speeds and variable (CR). The results suggested that CO₂ in biogas fuel greatly influenced the reduction of the toxic NO_x emissions and also enhance the SI engine in operating at a high CR. However, it is unfortunate to observe that incomplete combustion as evidenced by high emissions of THC was prominent in the presence of excessive amounts of CO₂. Meanwhile the emissions of CO remained unaffected by CR and crankshaft speed but CO correlation existed with the relative air-to-fuel ratio. Jung et al [37] studies suggested that biogas combustion in engines could be improved by increasing the methane percentage composition of the biogas. The study investigated the extension of lean operational limit up to a relative air/fuel ratio of 1:5 with variable biogas compositions and for CH₄: CO₂ volume ratios of up to 70%: 30 % with no engine knocking. The emissions of NO_x were reduced to near-zero due to the decrease in the combustion temperature, which was aided by use of the lean combustion mixture.

Bedoya et al [38] studied the effects of biogas composition on homogeneous charge compression ignition (HCCI) combustion system. They adopted a numerical methodological approach which combines chemical kinetics and CFD numerical simulation to analyse the trends in emissions and combustion parameters. They numerically analysed the effect of biogas fuel composition using the HCCI engine in terms of its combustion and emission parameters. Obtained results showed that NO_x emissions were not primarily influenced by biogas composition however, CO and non-combusted THC emissions increased with increase in the percentage composition of CO₂. The numerical results also indicated that biogas composition could be used as an effective way of controlling the onset of combustion as well as combustion phasing in biogas fuelled HCCI engines thus allowing for combustion stability and operational safety with low and high equivalence ratios. Abade [39] study numerically simulated CH₄/ CO₂ fuel mixture in order to investigate its effect on emissions and catalyst performance of a biogas-fuelled SI engine. The study revealed that increasing the CO₂ content led to a sharp increase in THC and a decrease in NO_x at the exhaust manifold. This concurred with the findings of Bedoya et al [38] study. Furthermore, it was noted in another study that doubling catalyst residence time will cause a rise in THC and CO emissions by a factor of 2. It was also noted that effective catalytic conversion of THC emissions depended more on the relative proportions of THC, NO_x and CO emissions at the level of the exhaust manifold [39]. Toppo [40] study presented a CFD model for an advanced combustion processes in CI engine. Temperature profiling inside the combustion chamber and NO_x emission at the exhaust manifold was compared for Jatropha fuel with conventional diesel fuel. The simulated results found were subjected to experimental validation for both Jatropha and diesel fuels in a CI engine system. The simulation was done in ANSYS- FLUENT code using non-premixed combustion modelling to imitate a real in-cylinder combustion phenomenon. Two-dimensional combustion system with mesh deformation was adopted in the simulation. The dimensions of the computational domain were aligned with the actual CI test engine. The findings of this study only revealed that the NO_x emitted for jatropha was more compared to that emitted by diesel. However, the study made no mention of a comparative study of biogas and diesel/petrol in terms NO_x emissions.

Noor et al [41] study presented a stepwise CFD simulation method for non-premixed moderate and intense low and diluted (MILD) oxygen biogas fuelled combustion furnace. A Non-premixed combustion model with a turbulent realizable standard *k*-epsilon was adopted in their simulation. The CFD simulation was achieved perfectly for the MILD regime and the maximum-to-average temperature ratio was found to be less than the expected 23%. Furthermore, it was also noted that meshing quality had optimum influence on convergence or divergence of calculations. Indicating that good CFD results is a product of high quality meshing achievable if and only if calculations converge. Vítázek et al [42] study was aimed at developing a new biogas mixture thermodynamics methodology using tabular exact parameters to calculate operating values of biogas composition. A biogas combustion mathematical model was developed and elaborated in addition to a simplified simulation diagram that was developed to depict the combustion device. The simulation diagram with indications of mass and energy movements was the kind, which would support the combustion of gaseous fuel as the limiting reactant. The findings revealed that using biogas directly proved difficult due to the presence of some H₂O, CO₂, N₂, H₂S, THC, organo-silicon compounds impurities. The presence of such impurities would make the potential of biogas usage as fuel to be costly due to additional purification cost.

Palaniswamy et al [11] used CFD software to investigate the maximum distance and optimal injector angle needed for a better biogas/air stoichiometric mixture at the intake manifold. Their findings indicated that the biogas introduced at 45° injector angle and 336mm distance from the axis of the inlet valve led to a better mixture. The experimentally validated results proved that 50% of blended biogas with a super-charged system was 25% more mechanically efficient compared to the natural aspiration system. The results also reported less CO emission values for a supercharged system.

Mameri et al [43] CFD simulation study revealed that the presence of CO₂ in biogas has a thermal dissociation effects. It absorbs energy from the combustion of methane, which leads to high exhaust temperature. The simulation study also showed convincingly that the useful energetic part of the biogas is methane. Therefore, suffice to say that biogas can be a better fossil fuel substitute provided CFD simulation feasibility studies are to be carried out prior to industrial implementation. Kuźnia et al [44] used a Chemked II program to model the biogas combustion kinetic process. The results of the study suggested that biogas combustion with greater CH₄ content does not necessarily lead to an increase in exhaust CO₂ gas concentration but rather improves engine performance.

Pablo [45] conducted an investigation using a diesel CI engine with a maximum output power 8.5 kW. The CI was converted into SI engine to allow gaseous fuel conditions and usage to be appropriate. In this study three fuel types were considered namely: simulated biogas, biogas (25% CH₄) and biogas (50% CH₄) by volume. The findings of this study suggested that CO₂ presence allowed the SI engine to operate at very high compression ratios (CR) even under usual combustion conditions. The study also found that enrichment of biogas with CH₄ resulted in an abrupt decrease in NO_x, CO and unburnt CH₄/THC emissions at the level of the exhaust manifold. This also concurred with findings from other studies [10, 37 – 39].

6. CONCLUSION

Carbon monoxide, sulphur dioxide, nitrogen oxides and particles are undesirable emissions associated with burning fossil fuels. The growing need to substitute fossil fuels with biogas for internal combustion engine particularly in automotive industry motivated the present study. This study successfully simulated and analysed previous studies focused on the fundamental impacts of firing biogas in an IC engine using CFD. From the study, it was gathered that the presence of CO₂ in biogas has a thermal dissociation effects during combustion in an IC engine. It absorbs energy from the combustion of methane, which leads to high exhaust temperature. The simulation study also showed convincingly that the useful energetic part of the biogas is methane. Also the present study revealed that using biogas directly proved difficult due to the presence of some H₂O, CO₂, N₂, H₂S, THC, organo-silicon compounds impurities. The presence of such impurities would make the potential of biogas usage as fuel to be costly due to additional purification cost. Therefore, suffice to say that biogas can be a better fossil fuel substitute provided CFD simulation feasibility studies are to be carried out prior to industrial implementation.

7. RECOMMENDATION

Computational work specifically using CFD simulation is now becoming more and more important due to its lower cost and acceptable accuracy with minimum error. A purely theoretical and numerical CFD simulation was employed in this study to investigate the combustion properties of biogas in an IC engine. The present study has shown that achieving unique operating conditions for biogas-fuelled engines, particularly in IC engines is not that simple. This is mainly due to the significant difference in biogas stoichiometric composition. Hence, an experimental investigation of biogas composition and its direct effect on emissions in IC engines should be carried out prior to its sole use as substitute for fossil fuel. From a South African perspective, the country has a large potential of biogas reservoirs whose energy can be exploited in the country's growing automotive industry. Hence, South Africa is perhaps better suited to explore the possibilities of utilising biogas energy as an alternative energy source especially for its automotive industry. In South Africa's automotive industry a drastic reduction in exhaust CO₂ concentration will go a long way in lowering greenhouse gas emissions.

ACKNOWLEDGMENTS REFERENCES

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