American Journal of Engineering and Applied Sciences

Original Research Paper

A Mathematical Modeling of the Turbulence Combustion Biodiesel in a Compression Ignition Engine: Theoretical Framework

[1,2]Francis Mouzong Bongne, [1,2,3]Zacharie Merlin Ayissi, [4]Bencher Mohamed and [5]Marcel Brice Obounou Akong

[1]Laboratory of Mechanics, Energiatronic and Sustainable Mobility (MESM), University of Douala, Douala, Cameroon
[2]Research Group in Strategy, Innovation and Sustainable Development (GRESIDD), National Polytechnic School of Douala (ENSPD) University of Douala, Douala, Cameroon
[3]National Polytechnic School of Douala (ENSPD) University of Douala, Douala, Cameroon
[4]Department of Mechanical Engineering, Faculty of Mechanical Engineering, University of Science and Technology "Mohamed Boudiaf" of Oran, Algeria
[5]Department of Physics, Energy, University of Yaoundé, Yaoundé, Cameroon

Article history
Received: 26-06-2024
Revised: 23-07-2024
Accepted: 01-08-2024

Corresponding Author:
Francis Mouzong Bongne
Laboratory of Mechanics, Energiatronic and Sustainable Mobility (MESM), University of Douala, Douala, Cameroon
Email: francismouzongbongne@yahoo.fr

Abstract: The present work proposes a new model for biodiesel combustion in an internal combustion engine. This model first includes the balance equations of gas dynamics with heat release. Secondly, a model with special properties that take into account turbulence effects is incorporated. The chemical models implemented in this study are for a biofuel used at less than 100% and for biodiesel-diesel blends. The resulting model is a coupling of equations describing the combustion of biodiesel with premixing. The model obtained is interesting and applicable to a wide range of combustion problems without major modifications. It is then proposed to the scientific community in order to develop internal combustion engines capable of meeting future political expectations regarding the reduction of pollutant emissions from the combustion of internal combustion engines.

Keywords: Turbulent Model, Biodiesel, Combustion, Mixing, Pre-Mixing

Introduction

The adverse effects of global warming, attributed mainly to greenhouse gas emissions, are having a considerable impact on the way we see the world and in particular on the use of energy resources. While a medium-term solution to the problem of pollutant emissions from the transport sector is awaited, internal combustion engines remain an effective means of logistics. A distinction is made between internal combustion engines (type I) and external combustion engines (type II). The two categories are distinguished by their mode of combustion. Type I engines burn within the engine, while type II engines burn outside. Type I engines are the most prevalent in the industrial sector.

One engine of this type whose performance is well-known is the diesel engine. They are the most sought-after for their adaptability and resistance to high combustion speeds (combustion with turbulence). Another major advantage of diesel engines is their ability to run on several types of fuel (diesel, biodiesel, biofuels, etc.). The performance of these engines with conventional fuels is well documented in the literature (Khoobbakht *et al*., 2019; Kibiwot *et al*., 2024). Nevertheless, the performance of these engines with biodiesel remains a subject of active research in numerous laboratories. The development of additional biofuels is underway with the objective of optimizing engines. However, in this context, it is of paramount importance to identify sustainable solutions for optimizing internal combustion engines, particularly those that respect the environment and guarantee human health. Heat engines are employed in motor vehicles to provide traction power.

Modeling represents a crucial element in the understanding of the physical processes involved. In contrast to experimentation, which may be more costly, modeling is preferred due to its relatively low financial cost. In order to gain a comprehensive understanding of the physical and thermodynamic processes involved, it is necessary to develop more comprehensive mathematical models with a minimal number of variables.

Several turbulence models have been developed for fuel combustion in diesel engines. Abdelrazek *et al*. (2023); Basevich *et al*. (2023); Gammaidoni *et al*. (2024). The main aim of these models is to reduce exhaust

emissions and improve engine energy efficiency. This was once done by the so-called experimental method (Yesilyurt, 2019; Kale and Krishnasamy, 2024). This alternative or complementary numerical method, which overcomes the indeterminacies of the experimental method, is the use of robust and powerful computer simulation techniques. It makes it easy to obtain reliable results at reduced time and cost. Computational Fluid Dynamics (CFD) has thus become an essential discipline for advancing engineering science in general and automotive engineering in particular. An alternative approach to direct numerical simulation of turbulent combustion of gas mixtures is suggested (Basevich *et al*., 2023). This model is based on the solution of the 3-dimensional transport equations for species concentrations and the energy conservation equation in a homogeneous, isotropic, and statistically stationary (forced) synthetic turbulence field at constant pressure. The detailed reaction mechanism is also considered (Basevich *et al*., 2023).

Recent fundamental advances in the modeling and computational power of the codes that have been set up reveal the greater attention that scientists and engineers are paying to CFD. Computational Fluid Dynamics (CFD) has a random and non-constant nature, making its prediction by the theoretical approach complex. The study of turbulence is therefore essential, as it plays a fundamental role in CFD. Taking turbulence into account means formulating assumptions about the transport process and establishing links between different physical parameters in the time-averaged flow (Li *et al*., 2024b; Özyalcin *et al*., 2024).

Several studies available in the literature propose the possibility of reducing pollutant emissions from engine combustion by using new combustion models. The study on the combustion properties, performance, and emissions of a single-cylinder diesel engine fueled with both diesel fuel and different volume percentages of Castor Methyl Ester (CME) has been exposed by Salman Edam and Al-Dawody (2019).

Aydın *et al*. (2020) developed an optimized artificial neural network model using response surface methodology when analyzing the performance and emissions parameters of a single-cylinder diesel engine fueled by biodiesel blends of formula C18H34 and pure diesel. The results obtained reveal that the proposed model correctly models exhaust emissions and performance parameters, with regression coefficients ranging from 0.8663-0.9858. The maximum mean relative error is less than 10% compared with experimental results. The response surface methodology demonstrated that a biodiesel content of 32% with an engine load of 816 W and an injection pressure of 470 bar are the optimum engine operating parameters. Postawa *et al*. (2024) investigated the feasibility of constructing artificial neural networks to predict feedstock and emission parameters from vineyard biomass combustion by implementing a novel dual artificial neural network model. The study showed that the final networks had a relative error of between 0.81-2.83% and the resulting dual neural network up to a maximum of 2.09%. Neural networks are also employed in the modeling of turbulent combustion in engines. In this approach, models derived from biological research are utilized to design computer architectures that can fulfill specific missions. Artificial neural networks have advantages and disadvantages (Baqer, 2024; Li *et al*., 2024a). These advantages include: Machine learning (they can learn from input data and adjust their weights to improve performance. This enables the model to be adapted to the specific characteristics of internal combustion engines), its ability to model complex relationships (they can capture non-linear relationships between variables, which is essential for modeling complex combustion processes, parallel processing (they can perform calculations simultaneously, speeding up processing time) and its adaptability (they can adapt to variations in operating conditions, which is crucial for internal combustion engines subject to varying loads and temperatures). Disadvantages include the heavy reliance on training data. Indeed, the performance of artificial neural networks is closely linked to the quality and quantity of the training data available. If the data is insufficient or biased, the model may not generalize correctly), and its complexity (the design and configuration of artificial neural networks requires expertise. Finding the right architecture and hyperparameters can be difficult, interpretability (artificial neural networks are often regarded as black boxes. Their decision-making is difficult to explain, which can pose problems in critical fields such as internal combustion engine combustion) and their sensitivity to outliers (artificial neural networks can be sensitive to outliers, which can affect their performance.

In order to accurately model combustion, it is essential to have a comprehensive understanding of the chemical processes involved. A chemical combustion process can be conceptualized as a sequence of cuts and bond creations between molecules (Williams, 1994). These cuts and/or bond creations represent elementary reactions, which constitute the kinetic reaction mechanism. The final stage of the reaction process corresponds to chemical equilibrium, which is defined by the laws of thermodynamics and the temperature and pressure conditions of this state. The mechanisms of chemical kinetics are numerous and are frequently utilized in various contexts.

García-Oliver *et al*. (2024) carry out a numerical analysis of 3D CFD simulations of fuel blends using the compact reaction mechanism approach involving 121 species and 678 reactions. The results show that the model

developed is capable of offering predictions that match the experimental result and can be used for diesel engine applications involving these promising fuels. Furthermore, numerical analysis highlights that a reduction of 50 and 37% respectively in soot and NOx emissions is achieved. The efficiency of diesel engines is also dependent on the geometry of the chambers. Therefore, it is necessary to consider the speed of combustion when conducting tests.

In their study, (Abdelrazek *et al*., 2023) used commercial Computational Fluid Dynamics (CFD) software combined with a chemical solver to model a direct injection diesel engine fueled by both base diesel and soybean biodiesel, performing a 3D numerical analysis at different loads. The renormalization group RNG coupled with a kinetic chemical reaction mechanism is used to model turbulence, combustion, and atomization. Respectively the proposed model adequately models the emission parameters, with a decrease in Carbon monoxide (CO) and Hydrocarbon (HC) emissions of about 42.38 and 41.35%, respectively, and an increase in Nitrogen Oxides (NOx) and Carbon Dioxide (CO) of about 21.8 and 11.2%, respectively. They conclude that biodiesel fuel can be used as an alternative and environmentally friendly fuel in the engine without any modifications. The renormalization group RNG is not adapted for engines having complex geometries. More generally, the model has limitations related to the physics of turbulent phenomena. However, some problems are turbulent. When solving complex confined or external combustions involving separation problems on irregular geometries, it is essential to maintain the positivity of these variables.

The choice of using a compact reaction mechanism depends on the specific needs of the simulation and the trade-off between accuracy and efficiency. This approach has both advantages and disadvantages (Abdelrazek *et al*., 2023; Jayabal, 2024). Advantages include: Energy efficiency (using a compact reaction mechanism enables chemical reactions to be modeled more efficiently, by reducing the number of chemical species and reactions to be taken into account. This simplifies calculations and enables results to be obtained more quickly, reduces computation time (by using a compact reaction mechanism, numerical simulations of internal combustion engine combustion are faster, which is essential for automotive engineering applications), and better performance prediction (compact reaction mechanisms are often based on experimental data and careful adjustments. They can provide more accurate predictions of engine performance, such as power, efficiency, and emissions). Disadvantages include Loss of detail (by simplifying the reaction mechanism, important details of specific chemical reactions can be lost. This can affect the accuracy of predictions, especially under extreme operating conditions), fuel specificity (some compact reaction mechanisms are specific to a fuel type or family. They may not be as generalized as more detailed mechanisms and adaptation to operating conditions (compact reaction mechanisms are often developed for specific operating conditions, for example, particular temperatures and pressures. They may not be as robust for variable conditions.

There are numerous turbulence models that have been utilized in the literature, each with its own set of advantages and disadvantages. Standard k-ε models are practical for internal flows, but they are not well-suited for complex flows with high-pressure gradients. SST k-w models are not suitable for transitional, compressible flows with complex geometries. These models tend to underestimate the transition position and overestimate separation. Herein, we propose a Reynolds-type k-ε model with the Boussinesq assumption. It is crucial to couple them with the fundamental gas dynamics equations. This enables their applicability to high-speed flows, where high combustion rates are desired.

Previous studies and many others show that the most widely used turbulence model is the standard k-ε, which gives better computational results far from the wall boundary. Its improved versions, the RNG k-ε which has improved accuracy for swirling flows, and the realizable k-ε model, the preferred model for circular and rotational turbulent flows are in great demand.

It is important to note that these models are often limited in their applicability to chambers with complex geometries. It is well established that combustion speed and, consequently, engine efficiency are highly sensitive to various parameters related to injection or chamber geometry. However, some of these models are unable to accurately predict combustion in complex flows with large pressure gradients and highly curved streamlines. In this study, we propose a combustion model that can be applied to any type of biodiesel (with different blend volumes), even with several chemical species. The model comprises fundamental equations, a k-ε Reynolds-type turbulence model and an integrated set of parameters optimally suited to diverse chamber geometries and even complex flows. In comparison with the models utilized in the literature, a reformulation has been implemented, which is now favorable regarding the model's pivotal parameters. Such a reformulation has led to a model that is ultimately associated with chemical kinetics. The resulting coupled model is applicable to a series of combustion processes with different flow regimes. Although it is adjustable, it is nevertheless capable of adapting to complex engine geometries.

The aim is to propose to the scientific community a new model of the turbulent combustion of biodiesel fuels in a premixed situation. We account for relevant parameters of

the turbulence via a positive *k-ε* model. The numerical tests of this model will be available in a future paper.

Materials and Methods

Mathematical Modeling

In this section, we propose the basis equations used in the modeling. To close these basis equations, we present a set of turbulent equations that are able to simulate combustion in an engine with accuracy. The idea is to create a model to evaluate the performance, combustion, and emissions of a single-cylinder diesel engine fueled with both pure diesel and diesel-abiodiesel blends containing Neem oil at various volumetric ratios.

Ideal-Gas Dynamic Equations

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0 \tag{1}$$

If we take into account contributions from the presence of chemical species:

$$\frac{\partial \rho}{\partial t} + \nabla(u\rho) = \dot{\delta}^s \tag{2}$$

Mass conservation or continuity equations for each species:

$$\frac{\partial \rho_m}{\partial t} + \nabla(\rho_m u) = \nabla\left[\rho D \nabla\left(\frac{\rho_m}{\rho}\right)\right] + f_m + \dot{\rho}_m^s + \delta_{m_1} \tag{3}$$

where, ρ_m represents the density of the species m, ρ the average density of the gas, u gas velocity, f_m is the source term due to chemistry and $\dot{\rho}_m^s$ is the source term due to liquid evaporation. Chemical species 1-2 correspond conventionally to fuel and oxidizer. Parameter D is the mass diffusion coefficient described by Fick's law of diffusion. δ is Dirac's delta function.

Equation of Momentum

It follows from Newton's second law, which states that the variation in momentum is equal to the sum of the forces acting on the fluid:

$$\frac{\partial(\rho u)}{\partial t} + \nabla.\rho(u \otimes u) = \nabla.(\tau - \overline{\rho u' \otimes u'}) + S_n \tag{3}$$

where, the viscous stress tensor is given by the following relationship:

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_i}\right) + \left(\mu' - \frac{2}{3}\mu\right)\left(\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) \tag{4}$$

In the above equations, u is the speed, ρ represents the density, S_n source term, p the pressure, μ the viscosity, μ' is the expansion viscosity (which is set to zero) and δ_{ij} is the Kronecker delta.

All these equations can be reduced to an equation of the form:

$$\frac{\partial \rho\phi}{\partial t} + \nabla.\rho(u\phi) = \nabla.(\Gamma_\phi \nabla\phi - \overline{\rho u'\phi'}) + S_\phi \tag{5}$$

where, can the value of any scalar? Reynolds constraints $\overline{\rho u' \otimes u'}$ and flow constraints $\overline{\rho u'\phi'}$ are the terms due to velocity fluctuations and represent convection effects.

Internal Energy Conservation Equation

It is derived from the first principle of thermodynamics:

$$\frac{\partial(\rho e)}{\partial t} + \nabla.(\rho u e) = -p\nabla.u - \nabla J + \rho\varepsilon + \dot{Q}^c + \dot{Q}^s \tag{6}$$

where, e is the specific internal energy, is the density, σ is the stress tensor, $and\ \dot{Q}^c$ and $\dot{Q}$ are source terms due to spray interactions and chemical heat, respectively. The heat flow vector J is the sum of contributions from thermal conduction and enthalpy diffusion.

Here, the internal energy e is given by Williams (1994):

$$\begin{aligned} e &= h - \frac{p}{\rho} \\ &= \int_{T_0}^{T} C_v dT - \frac{RT_0}{W} + \sum_{k=1}^{N} \Delta h_{f,k}^0 Y_k \\ &= \sum_{k=1}^{N} e_k Y_k \end{aligned} \tag{7}$$

Here, $\Delta h_{f,k}^0$ is the enthalpy required to form one kilogram of the species k. The fraction of the species k is given by: $Y_k = \frac{m_k}{m}, k = 1, \ldots, N$ the variable N corresponds to the number of species present in the reactive mixture, m_k is the mass of the species k present in a given volume V, and m total mass of gas in the volume V. The pressure $= \sum_{k=1}^{N} p_k, p_k = \rho_k \frac{RT}{W_k}$, with $\rho_k = \rho Y_k$ and W_k being respectively the density and molecular mass of the species. k. For a multi-species mix $\rho = \sum_{k=1}^{N} \rho_k$ and the perfect gas equation is given by $p = \rho \frac{RT}{W}$ where, W is the average molecular weight of the mixture given by: $\frac{1}{W} = \sum_{k=1}^{N} \frac{Y_k}{W_k}$. Here again, the specific C_v heat at constant volume of the mixture is represented by:

$$C_v = C_p - r\ with\ r = \frac{R}{W} = R\sum_{k=1}^{N} \frac{Y_k}{W_k} \tag{8}$$

and C_p the specific heat at constant pressure given by:

$$C_p = \sum_{k=1}^{N} C_{pk} Y_k, \tag{9}$$

where, C_{pk} is the species-specific heat at constant pressure k given by:

$$C_{pk} = 2.5\frac{R}{W_k} \quad (10)$$

The evolution of the mass fraction function of the rate of chemical depletion/production of the k[th] species reads:

$$\rho\frac{\partial Y_k}{\partial t} = \omega_k + \nabla.(D_k\rho\nabla Y_k) - \rho_0 U_0'\nabla Y_k, k = 1,\ldots,N \quad (11)$$

In the fresh mixture, the vector $U_0' = (u_0', v_0', w_0')$ represents the velocity fluctuations. The diffusion coefficient of k species is noted as D_k. The term ω_k (the rate of chemical consumption or production of species k) is given by Williams (1994):

$$\omega_k = \mu_k \sum_{k=1}^{M} (\gamma_{k,j}^- - \gamma_{k,j}^+) A_j T^{\alpha_j} e^{-\left(\frac{E_j}{R^0 T}\right)} \prod_{i=1}^{N} \left(\frac{X_i p}{R^0 T}\right)^{\gamma_{k,j}^+}, k = 1,\ldots N \quad (12)$$

With A_j the pre-exponential factor of the j^{th} reaction, $\gamma_{k,j}^-$ and $\gamma_{k,j}^+$ the stoichiometric coefficients, a_j the temperature exponent, E_j activation energy, X_i mole fraction of the species, and M is total the number of chemical reactions.

The Navier-stokes system of reactive equations (coupled with turbulence) requires an elementary reaction mechanism describing the physical and chemical basis of premixed turbulent combustion (a situation where a biofuel can be used at a certain percentage). The time scales of chemical reactions are generally smaller than the small time scales of turbulence, resulting in a highly complex, non-linear, coupled system of differential equations.

Chemical Model

Chemical Model for a 100% Used Biofuel

The rate of combustion and, consequently, the efficiency of the engine are highly susceptible to a multitude of parameters related to the injection or chamber geometry.

When biofuel burns without premixing, it changes from one chemical species to another. The reaction rate of change can be calculated by the following relationship:

$$\dot{\omega}_r = \frac{dY_m}{dt} = \frac{Y_m - Y_m^*}{\tau_c} \quad (13)$$

where, Y_m represents the fraction of the species, Y_m^* is the value of this fraction at thermodynamic equilibrium, $and\ \tau_c$ is the mixing time characteristic of equilibrium completion given by:

$$\tau_c = \tau_{chim} + f\tau_t \quad (14)$$

where, τ_{chim} represents the turbulent mixing time dependent on the perfect gas constant and the gas temperature; τ_t the turbulent mixing time given by $\tau_t = C_2\frac{k}{\varepsilon}$, $C_2 = 0.1, E = \frac{77.3KJ}{mol}$, E being the activation energy; the function $f = (1 - e^{-Y})/0.632$ is the parameter that simulates the decreasing influence of turbulence on the combustion process.

Chemical Model for a Biofuel Used Less than 100%

Elementary reactions are characterized by their reaction rate θ_i (or the variation of the species over time), which enables us to calculate the effect of the reaction on each species. We mention that the elementary reaction rate is equal to the product of a rate constant and the concentrations of the reactive species, each raised to a power corresponding to their stoichiometric coefficient. The rate constant depends on temperature and is usually expressed by an Arrhenius law:

$$r = BT^{\alpha}\exp(\frac{E_a}{RT}) = BT^{\alpha}\exp(-\frac{\tau_a}{T}) \quad (15)$$

where, r is the speed constant, B is the pre-exponential coefficient, R is the perfect gas constant, E_a activation energy, and $\tau_a = \frac{E_a}{R}$ activation temperature.

The activation energy represents the amount of energy required by the system under consideration for the species to react significantly. By comparing the characteristic lengths and times of turbulence with the characteristic lengths and times of laminar flames, we obtain a classification of turbulent flame structures. Two numbers can be used to establish this classification: That of Damkhöler D_a and the one of Karlovitz K_a. These numbers compare the chemical characteristic time τ_c at characteristic turbulence times τ_t and τ_D respectively associated with the energetic and dissipative structures of turbulence. These two numbers are linked by the Reynolds given by the following formula:

$$\mathrm{Re}_T = D_a^2 K_a^2$$

Turbulence Modeling

To close the above system of equations, we propose a Reynolds-type turbulence model with the Boussinesq hypothesis that is able to adapt to complex engine geometries. The model is also able to simulate transition positions accurately and to better estimate separations. Historically, several closure models have been developed to relate turbulent viscosity to kinetic energy (Wilcox, 2008). The flowchart in Fig. (1) presents the models developed, their components, and the position of the model proposed in this study. A "*turbulent viscosity*" model was selected and modified. Boussinesq's assumption that state that the Reynolds tensors $\overline{\rho u' \otimes u'}$ can be related to mean velocity and turbulent viscosity gradients in a manner analogous to that which relates stress and strain tensors to deformations in a Newtonian fluid was employed.

The Reynolds stresses read:

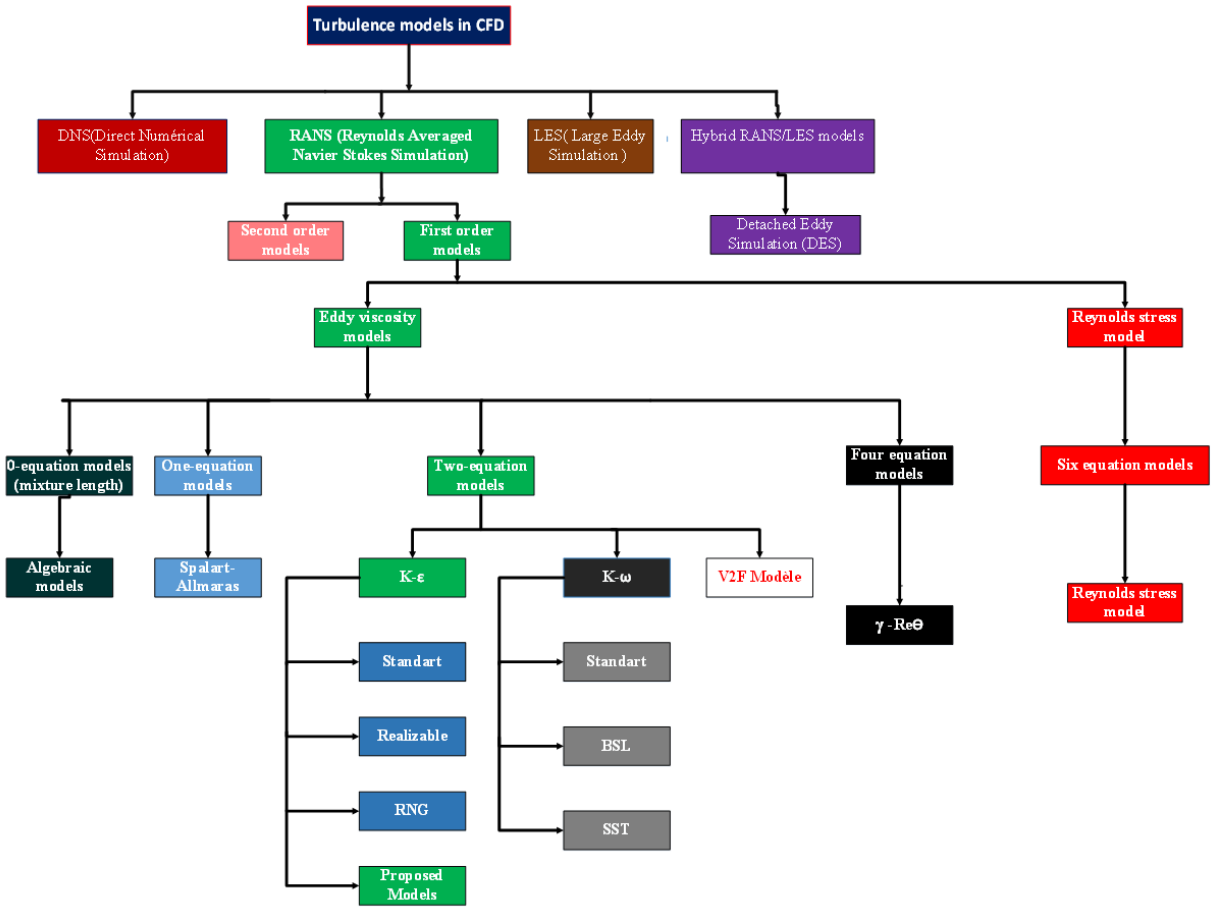

Fig. 1: Flowchart of different modeling available in the literature

$$-\overline{\rho u' \otimes u'} = \mu_t(\nabla u + \nabla u^t) - \frac{2}{3}\delta(\rho k + \mu_t \nabla . u) \quad (16)$$

μ_t is the turbulent viscosity to be modeled (often desired to be positive). We also define turbulent diffusivity, which assumes that the Reynolds fluxes of a scalar are linearly proportional to the mean gradients of that scalar:

$$-\overline{\rho u'\Theta'} = \Gamma_t \nabla \Phi \quad (17)$$

where, Γ_t is the turbulent diffusivity $\Gamma_t = \frac{\mu_t}{Pr_t}$, Pr_t the Prandtl number. In the model $k-\varepsilon$, we calculate μ_t as follows (Wilcox, 2008):

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \quad (18)$$

With K and ε respectively the kinetic energy and dissipation are given by: the kinetic energy equation of the kinetic energy of turbulence:

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla . \rho(u\varepsilon) = \nabla . [(\mu + \frac{\mu_t}{\sigma_\varepsilon})\nabla \varepsilon] + \frac{\varepsilon}{K}(C_{g_1} P_k - C_{g_2}\rho\varepsilon) \quad (20)$$

The energy dissipation rate equation is:

$$\frac{\partial k}{\partial t} + \nabla . \rho(uk) = \nabla . [(\mu + \frac{\mu_t}{\sigma_k})\nabla k] + P_k - \rho\varepsilon, \quad (21)$$

The term P_k represents the kinetic energy production of turbulence given by turbulence given by:

$$P_k = 2\mu_t tr(\Delta_{ij}) = 2\mu_t \Delta_{ij} \quad (22)$$

In the following, we will try to find laws for these new turbulence flows. $\left(\overline{\rho u' \Phi'}, \rho u' \otimes u'\right)$, just as it was necessary to find them for molecular diffusion fluxes, otherwise the new equilibrium equations are unusable. However, we recognize the inefficiency of the $k-\varepsilon$ to model certain types of flow and its capabilities have been unfairly called into question.

The model $k-\varepsilon$ has five closure coefficients, which are determined by replacing indeterminate double and triple correlations with algebraic expressions involving the properties of mean flow and turbulence. As the flow

is confined, we prefer to give these coefficients the following values (Wilcox, 2008):

$$c_{g_1} = 1.44; c_{g_2} = 1.92; c_\mu = 0.09; \sigma_k = 1; \sigma_\varepsilon = 1.3 \quad (23)$$

However, at the edge of the wall where viscosity effects dominate, the $k-\varepsilon$ no longer applies. We will therefore model the wall effect by the friction it imposes on the fluid and the velocity gradients will be calculated using the wall law.

Positivity of $k-\varepsilon$

We use logarithmic variables $(k=\hat{k}\ and\ \varepsilon=\hat{\varepsilon})$ representing practical solutions. To preserve the positivity of $k-\varepsilon$, considering $\nabla k = k\nabla\hat{k}, \nabla\varepsilon = \varepsilon\nabla\hat{\varepsilon}$, we obtain:

$$\frac{\partial\hat{k}}{\partial t} + \nabla.\left[\rho u\hat{k} - \left(\mu + \frac{\mu_t}{\sigma_t}\right)\nabla\hat{k}\right] = \left(\mu + \frac{\mu_t}{\sigma_k}\right)\nabla\hat{k}\nabla\hat{k} + e^{-\hat{k}}(p_k - \rho e^{\hat{\varepsilon}}) \quad (24)$$

$$\frac{\partial\hat{\varepsilon}}{\partial t} + \nabla.[\rho u\hat{\varepsilon} - (\mu + \frac{\mu_t}{\sigma_t})\nabla\hat{\varepsilon} = (\mu + \frac{\mu_t}{\sigma_k})\nabla\hat{\varepsilon}\nabla\hat{\varepsilon} + e^{-\hat{k}}(c_{g_1}p_k - c_{g_2}\rho e^{\hat{\varepsilon}}) \quad (25)$$

Through these two new equations, we can see that a new strongly non-linear term appears ($\alpha\nabla\hat{\varepsilon}\nabla\hat{\varepsilon}$) which could complicate convergence. Nevertheless, these equations make it easier to preserve the positivity of *k* and ε but also μ_t given this time if by:

$$\mu_t = c_\mu \rho e^{2k-\varepsilon} \quad (26)$$

The turbulent model for biodiesel combustion given by (23-26) is coupled with the chemical model and the ideal-gas dynamic equations.

Results and Discussion

The classical model $k-\varepsilon$ given by system of Eq. (20-21) has limitations related to the physics of turbulent phenomena. Standard k-ε models are practical for internal flows, but they are not well-suited for complex flows with high pressure gradients.

Most $k-\varepsilon$ turbulent models are not applicable when the strong gradient of kinetic energy. In addition, these models are unable to accurately predict combustion in complex flows with large pressure gradients and highly curved streamlines.

For example, the SST k-w models are not suitable for transitional, compressible flows with complex geometries.

When solving complex confined or external combustions involving separation problems on irregular geometries, it is essential to maintain the positivity of k and ε. While there are still schemes that preserve the positivity of these variables, these have drawbacks that can affect the convergence and accuracy of the solution. One solution to this problem of the positivity of k and ε is to solve their algorithm. We have proposed here an original reformulation that maintains positive these variables by letting $\nabla k = k\nabla k, \nabla\varepsilon = \varepsilon\nabla\hat{\varepsilon}$.

This strategy is justified by the behavior of k and ε which tend to change very quickly. As the logarithm grows slowly, its arguments help to improve the accuracy of solutions, particularly when k and ε have strong gradients.

The coupled model is an extension of those based on the classical $k-\varepsilon$ turbulent model used in several works in the literature. The classical turbulent models neglect several aspect as mentioned above. The developed $k-\varepsilon$ turbulent model are applicable when the strong gradients of kinetic energy arise. In addition, the models are able to accurately predict combustion in complex flows with large pressure gradients and highly curved streamlines. The $k-\varepsilon$ turbulent model for biodiesel combustion is better than the classical $k-\varepsilon$ models widely used and this is proved theoretically in this study.

The model is promising, but there is still room for improvement. It is possible to apply this model to a series of combustion processes with different flow regimes. Although it is adjustable, it is nevertheless capable of adapting to complex engine geometries.

Conclusion

In this study, we have proposed a model of biodiesel combustion in a single-cylinder engine. The model first includes the balance equations of gas dynamics with heat release. We then propose to introduce turbulence via a model of the type with specific properties. The chemical models for a biofuel used at less than 100% and at more than 100% are presented below. The resulting model is a coupling of equations writing biodiesel combustion with premixing. The model developed is interesting and can be applied to a wide range of combustion problems. Numerical experiments using finite volume methods on the model will be presented in a future investigation. Laboratory experiments will also be carried out.

Formulas for chemical models can be redesigned to better approximate biofuel combustion problems. The numerical tests will be available in a future paper. Future work will likely increase the size of the proposed modeling through the creation of a mechanism for larger biodiesel. This allows us to better represent biodiesel fuel and this represents added complexity. Thus concurrent efforts will be necessary to address the computational power required to utilize this model. Another way to address this issue of size and computational cost is mechanism reduction that leads to the suppress of some reactions that are not important in achieving certain

computational targets, such as species concentrations, or temperature profiles.

Acknowledgment

The author would like to thank an anonymous referee for giving very helpful comments and suggestions that have greatly improved this study.

Funding Information

The authors received no financial support or funding to report.

Author's Contributions

Francis Mouzong Bongne: Original draft of the manuscript, written, methodology, revision and edited, conceptualization, submission.

Zacharie Merlin Ayissi and Bencher Mohamed: Reviewed and edited, validation, supervision.

Marcel Brice Obounou Akong: Revision methodology and edited.

Ethics

This document is unpublished and original. The corresponding author certifies that all other authors have read and approved the manuscript, without any ethical concerns being involved.

References

Abdelrazek, M. K., Abdelaal, M. M., & El-Nahas, A. M. (2023). Numerical simulation of a diesel engine performance powered by soybean biodiesel and diesel fuels. *Beni-Suef University Journal of Basic and Applied Sciences*, *12*(1), 11. https://doi.org/10.1186/s43088-023-00349-w

Aydın, M., Uslu, S., & Bahattin Çelik, M. (2020). Performance and emission prediction of a compression ignition engine fueled with biodiesel-diesel blends: A combined application of ANN and RSM based optimization. *Fuel*, *269*, 117472. https://doi.org/10.1016/j.fuel.2020.117472

Baqer, I. A. (2024). Intelligent fault detection of spark plugs using vibration signal analysis and artificial neural networks. *International Journal of Vehicle Noise and Vibration*, *20*(1), 1–26. https://doi.org/10.1504/ijvnv.2024.138094

Basevich, V. Y., Belyaev, A. A., Frolov, F. S., & Frolov, S. M. (2023). Turbulent Flame Propagation in Hydrogen-Air and Methane-Air Mixtures in the Field of Synthetic Turbulence: Direct Numerical Simulation. *Eng*, *4*(1), 748–760. https://doi.org/10.3390/eng4010045

Gammaidoni, T., Miliozzi, A., Zembi, J., & Battistoni, M. (2024). Hydrogen mixing and combustion in an SI internal combustion engine: CFD evaluation of premixed and DI strategies. *Case Studies in Thermal Engineering*, *55*, 104072. https://doi.org/10.1016/j.csite.2024.104072

García-Oliver, J. M., Novella, R., Micó, C., Bin-Khalid, U., & Lopez-Pintor, D. (2024). A numerical analysis of hydrotreated vegetable oil and dimethoxymethane (OME_1) blends combustion and pollutant formation through the development of a reduced reaction mechanism. *International Journal of Engine Research*, *25*(6), 1174–1190. https://doi.org/10.1177/14680874231226321

Jayabal, R. (2024). Effect of hydrogen/sapota seed biodiesel as an alternative fuel in a diesel engine using dual-fuel mode. *Process Safety and Environmental Protection*, *183*, 890–900. https://doi.org/10.1016/j.psep.2024.01.046

Kale, A. V., & Krishnasamy, A. (2024). Experimental study on combustion, performance, and emission characteristics of a homogeneous charge compression ignition engine fuelled with multiple biofuel-gasoline blends. *Energy*, *288*, 129621. https://doi.org/10.1016/j.energy.2023.129621

Khoobbakht, G., Karimi, M., & Kheiralipour, K. (2019). Effects of biodiesel-ethanol-diesel blends on the performance indicators of a diesel engine: A study by response surface modeling. *Applied Thermal Engineering*, *148*, 1385–1394. https://doi.org/10.1016/j.applthermaleng.2018.08.025

Kibiwot, V. N. (2024). Modelling of engine performance and emissions fueled by biodiesel blends. *Editon Consortium Journal of Engineering and Computer Science*, *1*(1), 1–12. https://doi.org/10.51317/ecjecs.v1i1.458

Li, G., Yang, R., Zhen, H., Wang, H., Liu, H., Tang, Q., & Yao, M. (2024a). Data-driven propagation prediction of subsonic and supersonic turbulent jets by combining self-similarity analysis model and artificial neural network. *Applications in Energy and Combustion Science*, *17*, 100236. https://doi.org/10.1016/j.jaecs.2023.100236

Li, J., Ye, L., Gong, S., Deng, X., Wang, S., Liu, R., & Yang, W. (2024b). Review on the combustion progress and engine application of tailor-made fuels from biomass. *Renewable and Sustainable Energy Reviews*, *192*, 114242. https://doi.org/10.1016/j.rser.2023.114242

Özyalcin, C., Sterlepper, S., Roiser, S., Eichlseder, H., & Pischinger, S. (2024). Exhaust gas aftertreatment to minimize NOX emissions from hydrogen-fueled internal combustion engines. *Applied Energy*, *353*, 122045. https://doi.org/10.1016/j.apenergy.2023.122045

Postawa, K., Klimek, K., Maj, G., Kapłan, M., & Szczygieł, J. (2024). Advanced dual-artificial neural network system for biomass combustion analysis and emission minimization. *Journal of Environmental Management*, *349*, 119543. https://doi.org/10.1016/j.jenvman.2023.119543

Salman Edam, M., & Al-Dawody, M. (2019). Numerical Simulation for the Effect of Biodiesel Addition on the Combustion, Performance and Emissions Parameters of Single Cylinder Diesel Engine. *Al-Qadisiyah Journal for Engineering Sciences*, *12*(2). https://doi.org/10.30772/qjes.v12i2.587

Wilcox, D. C. (2008). Formulation of the kw turbulence model revisited. *AIAA Journal*, *46*(11), 2823–2838.

Williams, F. A. (1994). The Next 25 Years of Combustion Theory. *Combustion Science and Technology*, *98*(4–6), 361–366. https://doi.org/10.1080/00102209408935421

Yesilyurt, M. K. (2019). The effects of the fuel injection pressure on the performance and emission characteristics of a diesel engine fuelled with waste cooking oil biodiesel-diesel blends. *Renewable Energy*, *132*, 649–666. https://doi.org/10.1016/j.renene.2018.08.024