Mika Kavanto

0D/1D modeling methods of in-cylinder combustion

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Author: Mika Kavanto
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ABSTRACT:
This thesis was a literature review for 0D/1D modeling methods for in-cylinder combustion in internal combustion engines, focusing on their theoretical foundations, practical applications, and comparative performance.

The study categorized combustion models into non-predictive, semi-predictive, and predictive approaches. Non-predictive models, such as the widely used Wiebe function, offered simplicity and computational efficiency but lacked adaptability to complex combustion phenomena. Semi-predictive models integrate empirical data and machine learning techniques, such as artificial neural networks (ANN), to estimate burn rate parameters, which improved accuracy within the training range but limited generalization. Predictive models, including entrainment and fractal approaches, relied on phenomenological principles to simulate turbulence and flame propagation, providing physical fidelity and predictive relevance at the cost of increased calibration complexity and computational demand.

A comprehensive literature review highlighted advancements in modeling strategies for spark-ignition engines under diverse conditions, including alternative fuels and lean-burn operation. Results indicated that while non-predictive models remain suitable for preliminary analysis and control-oriented applications, predictive models offered greater physical fidelity for performance optimization and emissions prediction. Semi-predictive methods bridged the gap between simplicity and precision but required extensive datasets for robust implementation.

The findings emphasized the trade-offs between model complexity, accuracy, and computational efficiency, offering guidance for selecting appropriate modeling techniques in engine design and simulation.

KEYWORDS: combustion modeling, Wiebe function, predictive models, artificial neural networks, spark-ignition engines, 0D/1D simulation

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TIIVISTELMÄ:
Tämä kandidaatintutkielma on kirjallisuuskatsaus, jossa tarkastellaan 0D/1D-mallinnusmenetelmiä polttomoottorin sylinterissä tapahtuvan palamisen mallintamiseen. Työssä keskitytään näiden menetelmien teoreettisiin perusteisiin, käytännön sovelluksiin sekä niiden suorituskyvyn vertailuun.

Tutkimuksessa polttoaineen palamisen mallinnusmenetelmät jaettiin ei-ennustaviin, puoli-ennustaviin ja ennustaviin lähestymistapoihin. Ei-ennustavat mallit, kuten laajalti käytetty Wiebe-funktio, ovat yksinkertaisia ja laskennallisesti tehokkaita, mutta niiden mukautuvuus monimutkaisiin palamisilmiöihin on rajallinen. Puoli-ennustavat mallit hyödyntävät empiiristä dataa ja koneoppimistekniikoita, kuten neuroverkkoja, palamisnopeuden parametrien arviointiin. Tämä parantaa tarkkuutta koulutusdatan puitteissa, mutta yleistettävyys jää usein rajalliseksi. Ennustavat mallit, joihin kuuluu esimerkiksi entrainment- ja fraktaalimallit, perustuvat ilmiöpohjaisiin periaatteisiin turbulenssin ja liekin etenemisen mallintamisessa, tarjoten paremman tarkkuuden, mutta vaatien enemmän kalibrointia ja laskentatehoa.

Laaja kirjallisuuskatsaus toi esiin kehitystä sytytystulppamoottoreiden mallinnusstrategioissa erilaisissa olosuhteissa, kuten vaihtoehtoisia polttoaineita ja laihaseospolttoa tarkasteltaessa. Tulokset osoittivat, että ei-ennustavat mallit soveltuvat edelleen esianalyyseihin ja säätöpohjaisiin sovelluksiin, kun taas ennustavat mallit tarjoavat paremman tarkkuuden suorituskyvyn optimointiin ja päästöjen ennakointiin. Puoli-ennustavat menetelmät asettuvat näiden välimaastoon, yhdistäen yksinkertaisuuden ja tarkkuuden, mutta vaativat laajaa dataa luotettavan toiminnan takaamiseksi.

Tutkimustulokset korostavat kompromisseja mallien monimutkaisuuden, tarkkuuden ja laskennallisen tehokkuuden välillä, tarjoten suuntaa antavia ohjeita sopivien mallinnusmenetelmien valintaan moottorisuunnittelussa ja simuloinnissa.

AVAINSANAT: palamisen mallinnus, Wiebe funktio, ennakoivat mallit, keinotekoiset neuroverkot, kipinäsytytysmoottori, 0D/1D simulointi

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Abbreviations

0D	Zero-dimensional
1D	One-dimensional
AFR	Air Fuel Ratio
ANN	Artificial Neural Networks
BMEP	Brake Mean Effective Pressure
BSFC	Brake Specific Fuel Consumption
CFD	Computational Fluid Dynamic
CI	Compression-Ignition
CNG	Compressed Natural Gas
EGR	Exhaust gas recirculation
GPM	Gaussian Process Model
GT-Suite/GT-Power	Engine simulation software (Gamma Technologies)
HCCI	Homogeneous Charge Compression Ignition
HRR	Heat release rate
IMEP	Indicated Mean Effective Pressure
ISFC	Indicated Specific Fuel Consumption
MFB	Mass Fraction Burned
MAPE	Mean Absolute Percentage Error
MC	Main Chamber
PCC	Pre Combustion Chamber
PFI	Port Fuel Injection
RMS	Root Mean Square
RMSE	Root Mean Square Error
SI	Spark-Ignition
SOC	Start of Combustion
STC	Sequential Turbocharging
T-GDI	Turbocharged Gasoline Direct-Injection
VVA	Variable Valve Actuation
VVT	Variable Valve Timing

1 Introduction

In engineering, modeling involves developing and using the appropriate methods and equations to analyze critical features of the process. Modeling contributes significantly to engine engineering by deepening our understanding of processes through interdisciplinary approaches. It also helps identify key variables for experiments, predict engine behavior under various conditions, determine trends and tradeoffs, and, when accurate, optimize design and control. One of the most important models is in-cylinder combustion modeling for engine simulations. (Gu et al., 2022; Heywood, 2019)

Overall computation time of full engine cycle depends on the calculation speed of the combustion model (Gu et al., 2022). Physics-based engine combustion models can differentiate into four main categories which increase in complexity and computational demand: zero-dimensional (0D) single zoned models (thermodynamic models using ordinary differential equations without spatial details), quasi-dimensional multizone models (accounting for interactions between zones using thermodynamic principles), 0D/1D single zone (extending 0D models with 1D CFD for engine pipes and manifolds), and multidimensional models. The multidimensional models are also known as computational fluid dynamic (CFD) and can provide detailed geometric information based on governing flow equations. (Heywood, 2019; Tang et al., 2021)

The goal of this thesis is to introduce modeling methods for in-cylinder combustion, review their capabilities, and present results from previous research. CFD modeling is out of the scope of this thesis due to its complexity, instead the thesis focuses on the 0D/1D modeling. Additionally, predictive modeling methods are focusing on spark-ignition (SI) engines.

2 Methods of modeling in-cylinder combustion

Chapter 2 introduces the main approaches for modeling in-cylinder combustion. It briefly outlines non-predictive, semi-predictive and predictive models from theoretical perspective.

2.1 Non-predictive

Engine simulations often use the universal combustion profile as a calculation input, with the S-shaped mass fraction burned profile represented by the Wiebe function Heywood (2019). According to Heywood (2019) the burn rate profile is a calculation input when burn rate on engine design and operating parameters are not modeled. Such models are useful when predictions for a range of assumed burn rate profiles provide the required information, or when the burn rate profile is not critical to the problem or study. For example, when detailed modeling of combustion dynamics is not feasible due to computational constraints, engineers may use assumed burn rate profiles to estimate engine performance across different operating conditions.

The Wiebe function is a widely adopted mathematical model for characterizing combustion processes within internal combustion engines, particularly in compression-ignition (CI) and spark-ignition (SI) types. The model is based on radical chain reactions and links chain reactions to fuel reaction rate and provides information on mass fraction burned (MFB), in-cylinder pressure, cumulative heat release, and heat release rate. In SI combustion spark timing starts the combustion, while in CI combustion it is started by chemical kinetics. (Tang et al., 2021)

Several commercial software platforms utilize Wiebe functions for engine simulation purposes, including GT-Power, AVL's Boost, Wave, Lotus Engine Simulation Software, and Lab Internal Combustion Engine. The continued usage of the Wiebe function over five decades since its introduction emphasizes Wiebe functions simplicity and adaptability. It remains especially beneficial in engine research, where a straightforward combustion

model offering high computational efficiency is required as an input for more complex simulations. (Ghojel, 2010)

2.1.1 Single-Wiebe

The standard Wiebe function is expressed as:

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

where $x_b(\theta)$ is the mass fraction burned (MFB), θ is the crank angle, θ_0 is the crank angle at the start of combustion (SOC), $\Delta\theta$ is the combustion duration defined as the difference between SOC, θ_0, and the end of combustion, *m* is the form factor because it determines the shape of the combustion process curve, and *a* is the efficiency parameter because it controls the duration of the combustion process. Spark timing is usually associated with θ_0, with combustion duration $\Delta\theta$ there is no consensus, and for example $\Delta\theta$ can be defined as crank angle interval between 5% MFB and 95% MFB. The least squares method is commonly utilized to estimate the parameters *a* and *m*, by comparing the Wiebe function with the calculated MFB as the ratio of the cumulative heart release to the total heat release. (Liu & Dumitrescu, 2019)

Ignoring the early and last stages will not cause a relatively large error when confirming the Wiebe parameters because these stages contribute minimally to the overall combustion process and are often subject to measurement uncertainties. Therefore, it is reasonable to ignore the early and last stages of the combustion process when validating the Wiebe parameters. (Hu et al., 2017)

2.1.2 Double(multi)-Wiebe

The standard Wiebe function has shown ability to calculate the mass fraction burned (MFB) with good accuracy in conventional stoichiometric spark-ignition (SI) engines (Heywood, 2019). However, its accuracy decreases in scenarios where the combustion process exhibits significant variability. This is particularly evident in advanced combustion strategies such as homogeneous charge compression ignition (HCCI) and dual-fuel

combustion, both of which often present highly variable burn rates that the standard Wiebe function struggles to capture effectively (Yasar et al., 2008). The primary limitation arises from the Wiebe function's restricted range of shapes, making it difficult to match the diverse burn rate profiles encountered in these advanced strategies (Yasar et al., 2008). To address this challenge, researchers have turned to alternative models. For example, in a study of dual-fuel combustion by Hu et al. (2022), the double-Wiebe function was employed because it could more accurately fit combustion processes where two distinct combustion phases coexist.

Following equation is improved equation of the double-Wiebe function by (1):

$$x_b(\theta) = \lambda\left\{1 - \exp\left[-a_1\left(\frac{\theta-\theta_0}{\Delta\theta_1}\right)^{m_1+1}\right]\right\}$$
$$+(1-\lambda)\frac{1+sign(\theta-\theta_{0,2})}{2}\left\{1 - \exp\left[-a_2\left(\frac{\theta-\theta_0}{\Delta\theta_2}\right)^{m_2+1}\right]\right\}, \qquad (2)$$

where $\theta_{0,i}$ is the start of the fast (i=1) or the slow (i=2) combustion process and *sign*($\theta - \theta_{0,2}$) equals -1 if $\theta \leq \theta_{0,2}$ and equals 1 if $\theta > \theta_{0,2}$. As a result, x_b (θ) is associated to the fast-burn if $\theta \leq \theta_{0,2}$ and slow-burn if $\theta > \theta_{0,2}$. In most cases, the selected value of $\Delta\theta_i$ may may not match the actual stage duration, but it is not an issue since the efficiency parameter a_i will adjust it towards to the real combustion duration. First improvement is compared to standard Wiebe function is the fast and slow burning stages start at different times. In addition, double-Wiebe function introduces the signum function to ensure that the calculation uses the second Wiebe function only for crank angles higher than the start of the second combustion stage. (Liu & Dumitrescu, 2019)

2.2 Semi-predictive

The difference between non-predictive and semi-predictive combustion modelling is that in semi-predictive modelling Wiebe function inputs are calculated from different significant variables (i.e. engine speed, intake manifold pressure, spark timing, etc.) using artificial neural networks (ANN). (Gamma Technologies, 2024)

A neural network is a mathematical system consisting of multiple simple processing elements (i.e. neurons) densely interconnected, as shown in Figure 1. Primary engine control variables, including the ignition timing, the air-fuel equivalence ratio, and the engine speed, were set as model inputs. The machine learning field is divided into three datasets: training, validation, and test. The training dataset helps adjust the machine learning algorithm to its intended purpose, while the validation dataset evaluates the model's performance in predicting new data. (Huang et al., 2021)

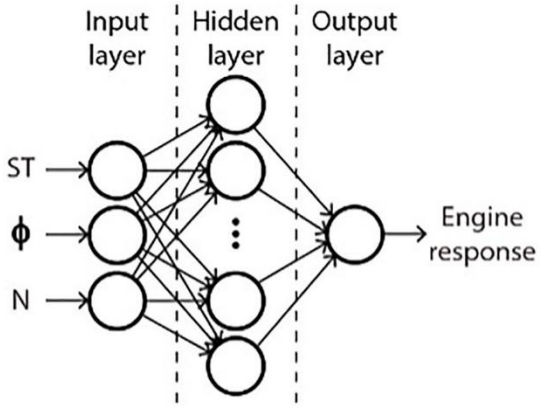

Figure 1. Schematic diagram of the artificial neural network model (Huang et al., 2021)

Dynamic artificial neural networks (ANN) are often trained to predict the steady-state characteristics of the engine combustion process within operating range of the training data set. Although it is less time consuming to develop an input-output model, as the combustion system becomes more sophisticated, the prediction capability of neural networks declines, if the numbers of neural network layers and nodes are not significantly increased. In this case, physics-based approach does have the advantage over the data-driven one. (Tang et al., 2021)

ANNs are powerful tools that simulate biological neural networks, combining inputs from various sources and performing non-linear operations on the result. These networks consist of three groups: an input layer, several hidden layers, and an output layer. The number of neurons in the input and output layers depends on the input and output experimental data. (Yusaf et al., 2010)

2.3 Predictive

In non-predictive combustion models, the burn rate is calculated as a function of the crank angle. It is independent of in-cylinder conditions assuming that there is sufficient fuel available. Factors such as residual fraction or injection timing do not affect the burn rate. If focus of the study is on these variables, for example non-predictive model is not suitable. (Gamma Technologies, 2024)

Various combustion models have been suggested for predicting the burn rate. With SI combustion models more widely used ones are based on the wrinkled thin reaction-sheet flame model. The winkled thin reaction-sheet flame model assumes that the overall flame approximates a portion of a sphere centered at or near the spark plug.
(Heywood, 2019)

2.3.1 Entrainment / eddy-burning

Keck et al. (1987) have derived entrainment-based burning law based on coupled analysis of flame front location and cylinder data that are shown on equations 3 and 4.
Rate of entrainment (laminar diffusion plus turbulent entrainment into the enflamed region):

$$\frac{dm_e}{dt} = \rho_u A_f s_L + \rho_u A_f u_T \left(1 - e^{-t/\tau_b}\right), \quad (3)$$

where ρ_u is the unburned gas density, A_f is the flame envelope area (portion of a sphere), S_L is the local laminar flame speed, u_T is the turbulent entrainment speed ($u_T \approx u'$), τ_b = (l_T / S_L) is the characteristic burning time, and l_T is the characteristic length scale of the turbulent fluid motion. First term in equation 3, represents the laminar diffusion of mixture across the approximately spherical front of the “thick” turbulent flame; the second term represents the entrainment of mixture into the flame due to the turbulent motion.

Rate of mixture burning (laminar flame propagation plus burn up of entrained yet-to-burn mass):

$$\frac{dm_b}{dt} = \rho_u A_f s_L + \frac{m_e - m_b}{\tau_b}, \quad (4)$$

In equation 4, the first term represents the burning due to the propagating laminar flame, and the second term the burn-up of unburned mixture within the turbulent flame "brush". This unburned mixture is the difference between the mass already entrained and the amount an already burned, contained within the "wrinkles" and "islands" which the distorting and stretching of the thin reaction sheet by the turbulent flow produce. This model is usually referred to as the "entrainment" or "eddy-burning" model for the reasons mentioned above. The exponential term within the brackets of the entrainment rate equation accounts that the flame sheet is initially spherical and "laminar-like": the flame sheet typically requires τ_b to transition into a turbulent flame.
(Heywood, 2019)

In figure 2 Heywood (2019) equations 3 and 4 are illustrated. The spherical front of the turbulent flame (dashed line) diffuses outward at the laminar flame speed S_L, and fresh mixture crosses this flame front at a characteristic velocity u_T due to turbulent convection. The schematic on left shows detailed flame structure: δ_L is the reaction-sheet thickness and l_T is the characteristic scale of wrinkles in flame sheet. (Keck et al., 1987)

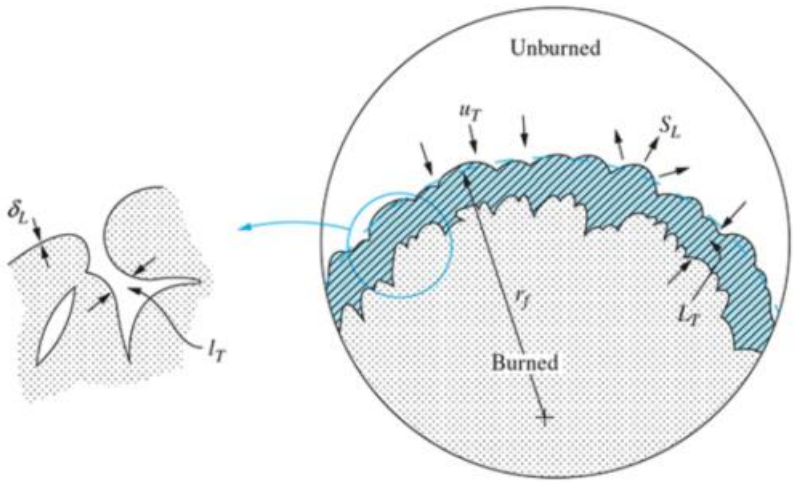

Figure 2. Schematic of turbulent premixed spark ignition engine flame illustrating the physical basis for the burning law of Equations 3 and 4. The approximately spherical front of the thick, turbulent flame. (Heywood, 2019)

2.3.2 Fractal model

Fractal combustion model presented in this chapter has been developed at the university of Naples "Federico II". The flame front propagating within the turbulent flow field is a thin, highly wrinkled surface resulting in a significantly increased flame area A_T compared to the smoot, spherical surface of laminar combustion centered at the spark plug. This increased flame surface area is the primary factor responsible for the higher turbulent burning rate relative to the laminar case. (De Bellis et al., 2017)

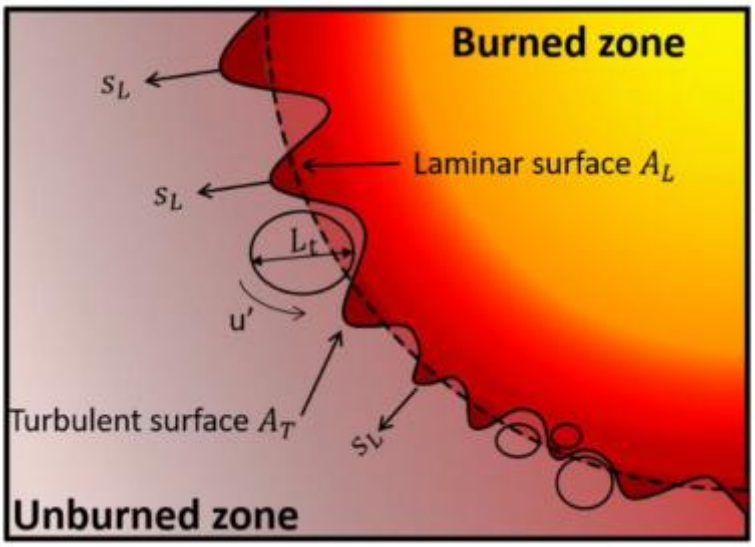

Figure 3. Schematic of the fractal combustion model (De Bellis et al., 2017)

In the fractal combustion model, the burn rate is expressed as:

$$\left(\frac{dm_b}{dt}\right)_{fractal} = \rho_u A_T S_L = \rho_u A_L \left(\frac{A_T}{A_L}\right) S_L, \quad (5)$$

where ρ_u, and S_L are same as in entrainment model, S_L is laminar flame speed, A_T is flame front turbulent area, and A_L is flame front laminar area. A_T/A_L is called as a wrinkling factor and comes from following equation:

$$\frac{A_T}{A_L} = \left(\frac{L_{max}}{L_{Gib}}\right)^{D_3-2} \left(\frac{L_{Gib}}{L_{min}}\right)^{(D_3-2)C_{d3}}, \quad (6)$$

where L_{Gib} is the Gibson scale, L_{max} is maximum wrinkling scale, L_{min} is minimum wrinkling scale, D_3 is fractal dimension, and c_{d3} is tuning constant. The Gibson scale can be calculated as a function of laminar speed and turbulence intensity that are previously presented and integral length scale L_t:

$$L_{Gib} = L_t \frac{{S_L}^3}{u'^3} \quad (7)$$

When the flame front is interacting with the combustion chamber walls, burn rate equation needs modifications. Although quasi-dimensional models cannot fully capture the complexities of flame-wall interaction, De Bellis et al. (2017) instead used a weighted average that combines the fractal burning rate with laminar wall combustion in following equations:

$$\frac{dm_b}{dt} = (1 - w_{wall})\left(\frac{dm_b}{dt}\right)_{fractal} + w_{wall}\left(\frac{dm_b}{dt}\right)_{wall} \quad (8)$$

$$\left(\frac{dm_b}{dt}\right)_{wall} = \rho_u A_L S_L \quad (9)$$

$$w_{wall} = \frac{A_w}{A_{tot}} {x_b}^{10x_{wc}} \ , \quad (10)$$

where progress variable w_{wall} defines the transition from turbulent to wall combustion through the ratio between A_w (the area wetted by the flame front on piston, head, and cylinder), and A_{tot} (the total flame front area). Wall combustion multiplier x_{wc} is another tuning constant. (De Bellis et al., 2017)

2.4 Summary of the methods

In non-predictive modeling Wiebe function is widely used to calculate the burn rate in combustion processes, with applications from predicting pressure and temperature to optimizing combustion in internal combustion engines. While the standard Wiebe function has been effective in certain cases, studies have shown its limitations in handling complex combustion processes. When multiple combustion phases are present, to accurately calculate the burn rate two or more Wiebe functions are needed. There is trade-off between model accuracy and computation time when increasing number of Wiebe functions. (Sun et al., 2017) Another limitation when using non-predictive models is that burn rate is imposed as a function of crank angle. Which means non-predictive models are not suitable when variables have direct or significant effect on burn rate. (Gamma Technologies, 2024)

Semi-predictive combustion model is sensitive to variables that have impact on burn rate but does not use physical models to predict the burn rate (Gamma Technologies, 2024). For example, Tarabet et al. (2014) used in their study ANN to predict Wiebe parameters based on input variables such as engine load and biodiesel blend. ANNs need large amounts of data for training and validation and to create accurate model (Yusaf et al., 2010). While utilizing ANNs offers prediction to burn rate, it is limited inside the range of training data used (Rajkumar et al., 2022).

Phenomenological based predictive combustion models do not impose burn rate like non-predictive models or being unreliable outside of training values like with semi-predictive models. Weaknesses of predictive models are amount of data to calibrate and validate the model and in addition, because of the complexity of the model's calibration process is more time consuming compared to the other methods. (Gamma Technologies, 2024)

3 Previous research results based on literature

Chapter 3 reviews variety of literature research of combustion models introduced earlier. For non-predictive modeling, only one study is discussed, as the Wiebe model is already extensively applied and well established in the literature due to its simplicity and versatility (Sun et al., 2017). Therefore, the focus of this chapter is on research articles related to semi-predictive and predictive modeling methods, which offer more advanced approaches for engine combustion analysis.

3.1 Non-predictive modeling study

Sun et al. (2017) present the development and validation of a combustion model for marine sequential turbocharging diesel engines, employing a double Wiebe function combined with the partial least squares method. The study utilized 142 operation points of a marine diesel engine with two sequential turbocharging (STC) systems, with 105 points for calibration and 37 for validation. The Wiebe combustion model was created to study STC system and develop STC control strategy. Utilizing numerical calculations reduces the need for extensive external environment testing that increases workload but also fuel consumption and pollutant emissions from extensive testing.

In the study Sun et al. (2017) used a double Wiebe function to simulate brake specific fuel consumption (BFSC) and pressure in different operation points of the STC systems. Seven Wiebe parameters were calculated using partial least squares regression (PLS-R). Combustion model was evaluated using statistical criteria such as coefficient of determination (R^2) and mean absolute percentage error (MAPE). R^2 values were above 0.99 between simulated and experimental results while MAPE of BSFC and maximum pressure parameters in all the calibration and validation points were 0.284% and 1.39% respectively. From the evaluation Sun et.al (2017) concluded that the model could accurately simulate engine performance and model could be used for creating reasonable control strategies for different STC systems.

3.2 Semi-predictive modeling studies

Chapter 3.2 reviews a selection of studies that have used semi-predictive modeling methods. The studies have been selected to cover variety of fuels and use cases.

3.2.1 Study on heavy-duty natural gas spark ignition engine

Huang et al. (2021) investigates the use of an artificial neural network (ANN) to model the performance and emissions of a heavy-duty natural gas spark ignition engine. The research utilized a single-cylinder CI engine that has been retrofitted for natural gas SI port fuel injection operation. The ANN uses engine control variables such as spark timing, mixture equivalence ratio, and engine speed were used as model inputs. Outputs for the ANN model were peak cylinder pressure, maximum pressure rise rate, indicated mean effective pressure, ignition lag, combustion phasing, burn duration, exhaust temperature and engine-out emissions. (Huang et al., 2021)

The model was trained using 80% of the experimental data, remaining data was used for validation. In addition, test dataset was selected from the validation set to evaluate if the model reproduced the relationships between the key control variables and engine responses. The model predicted engine responses with acceptable errors from the evaluation criteria, R^2 values larger than 0.9 and close to zero RMSE errors. Huang et al. (2021) have stated in study that values from the combustion phasing parameters (CA50, CA90 and combustion duration) could be used as an inputs for Wiebe function model. While model showed acceptable accuracy, no relationship between CA90 and operation variables was formed. In addition, there were difficulties building relationship between CO emissions and key operation variables, even with good evaluation values. (Huang et al., 2021)

Huang et al. (2021) concludes that the ANN model effectively simulated the nonlinear combustion process withing the operating range used for training. However, the model's performance outside the training range remains uncertain. Additionally, the model is

only applicable to the specific hardware combination on which it was trained. Despite these limitations, the study emphasized the potential of ML models as a powerful tool for engine analysis, sensitivity analysis, and optimization problems. (Huang et al., 2021)

3.2.2 Study on Methane-Hydrogen fueled engines

Molina et al. (2021) have developed a novel combustion modeling approach utilizing machine learning is proposed to predict the burning rate of various methane-hydrogen mixtures. In the research Molina et al. (2021) employs a single-cylinder version of a four-cylinder light-duty engine for automotive applications. Due to the high costs associated with hydrogen engine experiments, simulations are used to minimize the number of required experiments (Molina et al., 2021).

Molina et al. (2021) highlights the limitations of Wiebe functions to accurately model mass burned fractions under varying fuel or air-fuel mixture conditions. Fractal combustion models, which assume that turbulence increases the burning rate by expanding the flame surface, are extensively used in research due to their accuracy across a wide range of operating conditions. However, these models face challenges in estimating laminar flame properties when switching fuels or using fuel mixtures, limiting their applicability in exploratory studies. (Molina et al., 2021)

Artificial Neural Networks (ANN) are introduced to overcome these limitations by estimating laminar flame speed from the thermochemical conditions within the combustion chamber (Molina et al., 2021). In the study Molina et al. (2021) investigates implementation of a modeling approach that accurately estimates the burning rate of air-fuel blends in the combustion chamber, using a combination of existing combustion models and ANN. The target is to enhance the accuracy of combustion modeling across diverse operating conditions, air-fuel dilutions, and fuel types while maintaining computational efficiency (Molina et al., 2021).

A comprehensive database of 10,000 scenarios was generated using a one-dimensional laminar flame code. The inputs for the ANN include in-cylinder pressure and temperature, air-to-fuel ratio, exhaust gas recirculation (EGR) levels, and the percentage of hydrogen in the fuel blend. The model was validated in two stages: first, by coupling the new combustion modeling approach with virtual engine and validating it under steady-state conditions using a stoichiometric compressed natural gas (CNG)/air mixture; and second, by validating the laminar flame speed under various lean conditions with pure CNG, pure hydrogen and their mixtures. The study also utilized CFD models to estimate turbulent flame speed properties. ANN achieved following accuracy: RMS training error is 5.63×10^{-3} and RMS testing error is 6.04×10^{-3}. (Molina et al., 2021)

Virtual Engine was validated against one operating condition with pure methane in stoichiometric conditions. Simulations showed acceptable accuracy when comparing following parameters: CA10, CA50, CA90-10, HRR, IMEP, ISFC, and indicated efficiency. When ANN model was compared against original model, the ANN model presented better accuracy with in-cylinder pressure and HRR. (Molina et al., 2021)

Despite the promising results, Molina et al. (2021) acknowledges certain limitations with the ANN model. Quantitative validation is required across a broader range of operating conditions, including different engine speeds, loads, and dilution conditions using exhaust gases. Additionally, cycle-to-cycle variation must be estimated to accurately predict losses due to excessive misfiring at high dilution rates. (Molina et al., 2021)

3.2.3 **Study on hydrogen-added combustion process in T-GDI engine**

Cho & Song (2020) investigates the prediction of the hydrogen-added combustion process in a turbocharged gasoline direct injection (T-GDI) engine using an artificial neural network (ANN). The ANN requires substantial data to generate accurate predictions which were obtained through simulations using 1D engine simulation software GT-Power. The GT-Power model, validated against experimental results, served as the basis for training Wiebe combustion model, where the Wiebe parameters were calculated

utilizing the ANN. Comparison between the ANN model and experimental results demonstrated reasonable accuracy, highlighting the potential of ANN as a solution for predicting combustion processes under various operating conditions. (Cho & Song, 2020)

The research methodology involved several steps. Engine experiments to create an accurate GT-power model. The GT-Power model uses SI turbulence model which is based on the predictive entrainment model. The predictive model was validated against 12 experimental cases. With the predictive GT-Power model a total of 15,000 cases were calculated which were used to train the ANN model. (Cho & Song, 2020)

The ANN was used to calculate Wiebe parameters: crank angle at 50%, duration for 10 – 90 % of the burned fuel (BD), Wiebe exponent, and combustion efficiency. Input parameters for the ANN were following mass flow rate of gasoline, hydrogen fraction, mass flow rate of air, spark timing, intake-/exhaust valve timing, and SOI (Cho & Song, 2020). The ANN model in study of Cho & Song, 2020 showed acceptable agreement with experimental data in both the mass fraction burned (MFB) profile and in-cylinder profile. Cho & Song, 2020 highlighted the potential of ANN for predicting the combustion process, achieving higher accuracy with more training data and greater versatility under a wider range of operating conditions. According to Cho & Song, 2020 combining experiments and simulations, it is possible to achieve good accuracy and versatility.

3.2.4 Study on diluted ethanol and methanol combustion

In their study Mahendar & Erlandsson (2021) focuses on the semi-predictive modelling of diluted ethanol and methanol combustion in conventional spark ignition operation, utilizing the SITurb combustion model. Although Mahendar & Erlandsson (2021) describe the method as semi-predictive, the SITurb model is inherently a predictive combustion model as it is based on the entrainment model. The primary objective in study by Mahendar & Erlandsson (2021) is to assess and enhance the accuracy of the SITurb combustion model available in GT-Power for diluted alcohol combustion. An experimental dataset was generated for ethanol and methanol using a single-cylinder heavy-

duty engine with a central spark plug and port fuel injection, achieving an IMEP of over 25 bars from a stoichiometric mixture up to an excess air ratio of 1.8. The engine, based on the Scania D12 was tested with 17 points for methanol and 16 points for ethanol, varying IMEP and excess air ratio. (Mahendar & Erlandsson, 2021)

Mahendar & Erlandsson (2021) identified that the GT-Power default laminar flame speed model underpredicts at higher excess air ratios, necessitating the use of an improved laminar flame speed correlation for ethanol and methanol. This correlation was developed using a chemical kinetics mechanism. At lambda of 1.4 and above, significant differences between the laminar flame speed models became evident. Despite improvements, the model underpredicted compared to experimental results, particularly at higher excess air ratios where the error in IMEP progressively increased. The SITurb model's sensitivity to turbulence levels, engine speeds, combustion phasing, and dilution allows for a wider simulation boundary compared to the Wiebe model. By incorporating the improved laminar flame speed model and dilution factor, the study demonstrates that diluted combustion can be predicted based on available stoichiometric test results. These results can assist to estimate the load limits, burn duration and efficiency that can be expected with alcohol fuels. (Mahendar & Erlandsson, 2021)

The default turbulence model introduced errors in burn rate calculations, and the default laminar flame speed model proved unsatisfactory at higher dilution levels. At a lambda of 1.8, combustion initiation was delayed, leading to significant errors in IMEP and CA10-75. The improved laminar flame speed correlation enhanced accuracy, reducing ignition delay to ±3 CAD across all excess air ratios. However, the combustion model continued to underpredict burn rates at lambda 1.6 and 1.8, with the default model failing to capture turbulent flame speeds at these points. (Mahendar & Erlandsson, 2021)

3.3 Predictive modeling studies

Chapter 3.3 focusses on reviewing studies in predictive combustion modeling methods. Like in previous chapter, the studies have been selected to cover variety of fuels and engine designs.

3.3.1 Study on prechamber-ignited lean-burn gas engine

Study by Accurso et al. (2022) focuses on the numerical simulation of a prechamber-ignited lean burn gas engine using predictive combustion models. The primary objective is to evaluate the predictive capabilities of the GT-Suite 0D/1D simulation software for a lean-burn gas engine equipped with an active PCC that uses a near-stoichiometric air-fuel mixture. This configuration allows rapid flame propagation and a rapid increase in pressure upon spark ignition. (Accurso et al., 2022)

Accurso et al. (2022) employs two distinct combustion models: one for the PCC and another for the main chamber (MC). The PCC combustion utilizes the SITurb combustion model (predictive entrainment model), while the MC combustion simulation employes the Jetignition model, originally designed for Turbulent Jet Ignition (TJI) combustion. Main idea in Jet ignition model is to describe the combustion process as a superposition of a jet combustion and flame combustion contribution. (Accurso et al., 2022)

Three different PCC geometries are investigated. The first geometry features a mixing volume with both spark plug, and gas admission pipe located on top, connected to the PCC holes via duct with lower diameter. The second geometry increases the diameter of both the connecting duct and the PCC holes by 15% and 20% respectively, compared to first geometry. The third geometry adopts a tapered shape for the mixing volume, eliminating the connecting duct and reducing the hole diameters while maintaining a similar total area due to an increased number of holes. This design reduces the total volume by 15% compared to first geometry. (Accurso et al., 2022)

GT-Suite model was calibrated by using experimental data from the first PCC. Other PCC geometries were then used to validate the calibrated predictive model to highlight the model's capabilities (Accurso et al., 2022). From the results Accurso et al. (2022) showed that reliable results were achieved without doing any specific optimization, only outlier was PCC #2 during low gas quantity, where simulations underestimate both maximum pressure in MC and HRR.

Accurso et al. (2022) concluded that proposed engine model can be used for performance and emission analysis of PCC-ignited gas engines. Model can be also used to carry virtual calibration activities of the engine, and preliminary analysis of PCC geometries (Accurso et al., 2022).

3.3.2 Study on Ultra-Lean Spark Ignition Engines

Sok et al. (2019) focuses on evaluating a predictive combustion model using a 0D/1D simulation tool under various conditions, including high load, different excess air ratios, and varying combustion stabilities. The experimental setup involves a single-cylinder, long-stroke, and flat-piston research engine, utilizing a five-component gasoline surrogate fuel. The model calibration was performed using 18 cases of experimental data, with engine operating at 1000 RPM using 500 cycle-averaged in-cylinder pressure data to optimize model constants. (Sok et al., 2019)

Sok et al. (2019) employs the SITurb model, combined with a newly developed phenomenological turbulence model based on 3D-CFD results. The built-in laminar flame speed function was found unsuitable for the use case, leading to the adoption of an improved laminar flame speed function based on the equations by Gülder and Megalchi & Keck. This revised laminar flame speed correlation was validated with six cases. Additionally, sensitivity analysis was done for three cases (high IMEP cycle averaged, averaged IMEP cycle, and low IMEP cycle averaged). Predictive model showed its effectiveness in predicting combustion under various stoichiometric-to-ultra-lean mixtures by calibrating only one combustion model parameter. (Sok et al., 2019)

Sok et al. (2019) concluded that combustion model using the improved laminar flame speed model shows less variation and complexity in calibration parameters compared to the default laminar flame speed model. The in-cylinder pressure and burn rate are reasonably replicated, and combustion characteristics such as CA50, CA10-90, maximum in-cylinder pressure and its location achieve a satisfactory accuracy (Sok et al., 2019).

3.3.3 Study on CNG SI Engines using 1D Simulation Tools

Riccardi et al. (2020) focuses in the study on enhancing the combustion model of natural gas spark ignition (SI) engines for 1D simulation tools. The study involves a SI engine retrofitted for compressed natural gas (CNG) use, utilizing a combustion model based on a fractal approach. A total of 25 cases were examined, with the primary objective being the validation of the combustion model. The model was calibrated under full load conditions to minimize the overall speed-average error between simulation and experimental combustion characteristics. Three tuning constats were specified, addressing different stages of combustion: the transition from initially laminar to fully turbulent combustion, the fully developed flame wrinkling, and the combustion tail. Through a trial-and-error procedure, a single set of tuning constants were identified and validated against the 25 cases. (Riccardi et al., 2020)

The results from Riccardi et al. (2020) study indicate that combustion model performs satisfactorily without case-dependent tuning, it demonstrates good performance even at part-load operating points. Validation was done against experimental air flow rate, with a low root mean squared error (RMSE) of 10.27 kg/h and all analyzed points falling within an error band of ±5% band. The model also showed low RMSE values for various combustion metrics, including 0.47 CAD for MFB10, 1.21 CAD for MFB90, and 2.86 CAD for experimental spark advance. Despite slight underestimations at low load and overestimations at high load the model's predictions of peak pressure and brake specific fuel consumption (BFSC) were within acceptable error margins. The RMSE for peak pressure was 1.22 bar, and for BSFC 5.85 g/kWh. It was noted that even better results are expected if more detailed tuning of turbulence sub-model is made. (Riccardi et al., 2020)

3.3.4 Study on comparing two combustion models with different SI Engines

De Bellis et al. (2017) presents a comparative analysis of two phenomenological combustion models, entrainment and fractal, which are applied to different spark-ignition (SI) engines. Both models demonstrate similar levels of accuracy, reliability, and applicability across various engines and operating conditions. However, the fractal model shows easier calibrating efforts and slightly better predictivity. The study initially involves three SI engines with distinct architectures, displacements, injection systems, and boosting mechanisms: a downsized turbocharged PFI VVA twin-cylinder engine (engine A), a high-performance VVT 10-cylinder naturally aspirated engine (engine B), and a DI high-performance turbocharged VVT 12-culinder engine (engine C). (De Bellis et al., 2017)

Dedicated experimental campaigns were conducted to calibrate and validate the models, acquiring main performance parameters with the in-cylinder pressure cycles. Post-processing was performed to derive burn rate profiles and combustion angles, specifically the mass fraction burned (MFB) at 10%, 50%, and 90%. Both models were coupled with the same laminar flame speed model and turbulence sub-model, and simulations were performed using GT-Power. Sensitivity analysis revealed that while the fractal model has a higher number of tuning constants, they can be straightforwardly identified, whereas the entrainment model requires time-consuming trial and error loops due to coupling effects. (De Bellis et al., 2017)

The combustion model assessment showed that both models were calibrated for each engine at full load, using global performance parameters such as volumetric efficiency, brake mean effective pressure (BMEP), brake specific fuel consumption (BSFC), and in-cylinder peak pressure. The study primarily focused on BMEP and BSFC comparisons, which showed good agreement with a percent error of 1-2% in most operating conditions, and always below 6% in the worst cases. When comparing MFB with mean squared error, the entrainment model performed better for MFB10 in Engine A, while

fractal model showed better results for MFB50-90 in Engine B and Engine C. (De Bellis et al., 2017)

Overall, both models predicted satisfactory accuracy compared to experimental data, with the fractal model showing slightly better agreement, particularly in reproducing the overall burn rate shape and combustion phase. The fractal model also demonstrated better capability to perceive the engine speed impact on the combustion process and required reduced tuning effort. An additional engine, labelled as engine D, was included as a blind test to further assess the models' strengths, with the fractal model showing slightly better accuracy. (De Bellis et al., 2017)

3.3.5 Study on modeling hydrogen combustion for heavy-duty applications

Rezaei et al. (2021) investigates in their study the numerical and experimental aspects of hydrogen combustion for heavy-duty applications, focusing on a hydrogen-powered single-cylinder test rig for a 2-liter heavy-duty engine. A combustion model based on entrainment approach was developed using hydrogen-specific sub-models to calculate laminar flame speed and auto-ignition in the unburned mass zone. The model was built in the GT-Suite simulation software to validate and evaluate the properties of hydrogen as a fuel for internal combustion engines, with results validated using experimental data. A novel mathematical approach for calculating laminar flame speed and an integrated auto-ignition model increased the accuracy of the simulation results. (Rezaei et al., 2021)

Additionally, Rezaei et al. (2021) investigates the suitability of the GT-Suite entrainment models' sub-models, focusing on turbulent and laminar flame speeds. The simulation of simple mixture enleanment at constant engine speed and load revealed significant over-estimation of the effect of excess air on flame propagation, resulting in prolonged burn durations at lean conditions. The calculated laminar flame speed approached zero, rendering the hydrogen-air mixture in the cylinder incombustible. The study found that the turbulent flame speed model did not affect the maximum air-fuel ratio (AFR) at which

combustion occurs, highlighting greater impact of laminar flame speed when accurately modelling fuel-specific effects. (Rezaei et al., 2021)

A Gaussian Process Model (GPM) was selected for its high flexibility and satisfactory accuracy in estimating laminar flame speeds across a wide range of operating conditions. Polynomial models failed to accurately estimate laminar flame speeds due to instabilities in certain boundary regions. The GPM, a probabilistic non-parametric model, accounts for anomalies in the data and provides prediction uncertainties, highlighting areas where prediction quality is poor due to a lack of data. The model training, performed with IAV Kasai software, involved simulating 1D laminar flame propagation at various boundary conditions using the latest version of the San Diego mechanism. The GPM approach achieved and average relative model error of less than 5%, with maximum relative errors lower than 10%. (Rezaei et al., 2021)

The calibrated hydrogen combustion model utilizing improved laminar flame speed model was validated at over 130 operating points, demonstrating its capability to accurately predict engine operation parameters and combustion characteristics. The model also serves as a solid foundation for the reliable simulation of engine-out NOx emission with the extended Zeldovich mechanism. The prediction error did not exceed 5% for parameters such as IMEP, λ, total EGR rate, BSFC, and maximum pressure, with MFB50, spark timing, and burn duration well within the predefined accuracy limit of 3°CA. (Rezaei et al., 2021)

4 Discussion

Non-predictive models, particularly the Wiebe function, are widely used due to their simplicity and computational efficiency. They are most effective when a straightforward representation of the combustion process is sufficient, such as in preliminary engine simulations or as input for more complex models. However, their main limitation lies in their inability to account for variable operating conditions or complex combustion phenomena, as the burn rate is imposed rather than predicted from physical parameters.

Semi-predictive models, which integrate empirical data and machine learning techniques like artificial neural networks (ANNs), offer improved adaptability and accuracy within the range of training data. Studies on heavy-duty natural gas spark ignition engines and methane-hydrogen fueled engines show that ANNs can effectively simulate nonlinear combustion processes and estimate key parameters such as laminar flame speed and burn duration. Nevertheless, these models are limited by the scope of their training datasets and may struggle to generalize beyond the conditions for which they were calibrated.

Predictive models, such as entrainment/eddy-burning and fractal approaches, provide the highest physical fidelity by simulating combustion based on engine and fuel properties. Research on prechamber-ignited lean-burn gas engines, ultra-lean spark ignition engines, and hydrogen combustion for heavy-duty applications demonstrates that predictive models can reliably reproduce experimental results and support advanced engine design and optimization. However, these models require substantial data for calibration and validation, and their complexity leads to increased computational demands.

5 Conclusion

Based on this study, the following conclusions can be drawn:

- The thesis reviewed and compared non-predictive, semi-predictive, and predictive methods for modeling in-cylinder combustion in engines.
- Non-predictive models, such as the Wiebe function, offer simplicity and computational efficiency but are limited in handling complex combustion processes and variable operating conditions
- Semi-predictive models improve adaptability by incorporating empirical data and machine learning techniques, but their accuracy is restricted to the range of training data and requires substantial data for calibration.
- Predictive models provide physical fidelity, simulating combustion based on engine and fuel properties, but demand more data and computational resources for calibration and validation.
- The choice of modeling method should be guided by the specific requirements of the engine simulation task, considering factors such as desired accuracy, available data, and computational constraints.
- Future research should focus on improving model calibration techniques, expanding validation datasets and integrating advanced machine learning approaches to enhance predictive capabilities.

6 Summary

This thesis examined the principal methods for modeling in-cylinder combustion in internal combustion engines, with a focus on 0D and 1D approaches. Non-predictive models, such as the Wiebe function, were found to offer simplicity and computational efficiency but are limited in handling complex combustion phenomena and variable operating conditions. Semi-predictive models, which incorporate empirical data and machine learning techniques, improve adaptability and accuracy within the range of training data, while predictive models provide the highest physical relevance and accuracy by simulating combustion based on engine and fuel properties, albeit with greater data and computational demands.

The literature review and comparative analysis highlighted that the choice of modeling method should be guided by the specific requirements of the simulation task, considering factors such as desired accuracy, available data, and computational constraints. The thesis concludes that future research should focus on improving model calibration, expanding validation datasets, and integrating advanced machine learning to further enhance predictive capabilities in combustion modeling.

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