# DEVELOPMENT OF A TWO ZONE TURBULENCE MODEL AND ITS APPLICATION TO THE CYCLE-SIMULATION

by

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*The development of a two zone k-ε turbulence model for the cycle-simulation software is presented. The in-cylinder turbulent flow field of internal combustion engines plays the most important role in the combustion process. Turbulence has a strong influence on the combustion process because the convective deformation of the flame front as well as the additional transfer of the momentum, heat, and mass can occur. The development and use of numerical simulation models are prompted by the high experimental costs, lack of measurement equipment and increase in computer power. In the cycle-simulation codes, multi zone models are often used for rapid and robust evaluation of key engine parameters. The extension of the single zone turbulence model to the two zone model is presented and described. Turbulence analysis was focused only on the high pressure cycle according to the assumption of the homogeneous and isotropic turbulent flow field. Specific modifications of differential equation derivatives were made in both cases (single and two zone). Validation was performed on two engine geometries for different engine speeds and loads. Results of the cycle-simulation model for the turbulent kinetic energy and the combustion progress variable are compared with the results of 3-D computational fluid dynamics simulations. Very good agreement between the turbulent kinetic energy during the high pressure cycle and the combustion progress variable was obtained. The two zone k-ε turbulence model showed a further progress in terms of prediction of the combustion process by using only the turbulent quantities of the unburned zone.*

Key words: *internal combustion engine, turbulence modeling, quasi-dimensional model, fractal combustion model, cycle-simulation*

## Introduction

In-cylinder flows of internal combustion engines are always turbulent due to the complex geometries and dynamic boundary conditions. Understanding the flows within the cylinder is a necessary step in the prediction of performances of spark ignition (SI) and compression ignition (CI) engines. The turbulent flow field inside the SI engine combustion chamber greatly influences the rate of heat release, the air-fuel mixing and stratification and the formation of pollutants; therefore, it has a great influence on the engine thermal efficiency [1-3].

The demand for turbulence modeling comes as a consequence of increased demand for quasi-dimensional combustion models which require an accurate prediction of the turbulent flow field inside the combustion chamber [4-7]. Various turbulence models for the simulations of SI engines have been developed and analyzed in the last few decades. The $k$-$\varepsilon$ turbulence

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model has often been used, including different modifications to equations for compressibility effects [8-10]. Tabaczynski [9] showed that the piston geometry can significantly change the evolution of the turbulent kinetic energy ($k$) during the high pressure cycle (HPC). Ramos [8] applied two different turbulence models, the full $k$-$\varepsilon$ turbulence model and the algebraic $\varepsilon$ model, to the same engine geometry. The results were analyzed but they were not validated with experimental data. Agarwal *et al.* [6] showed different single and two zone turbulence model formulations (algebraic $\varepsilon$ model and $k$-$\varepsilon$ turbulence model) which were applied to the quasi-dimensional SI combustion model. In all the work mentioned above, the turbulence model coefficients are calibrated by the experimental results of the in-cylinder pressure. The turbulent kinetic energies obtained by different models have been analyzed and compared, but they have not been compared with experimental or CFD results. The overall structure of the quasi-dimensional SI combustion model contains a turbulence model and a model that calculates the burned mass fraction based on the calculated turbulence intensity. Calibration of turbulence coefficients based on the in-cylinder pressure can produce different turbulence profiles during combustion, with different combustion model coefficients.

This paper presents the continuation of the previous work where a single zone $k$-$\varepsilon$ turbulence model and its implementation in cycle-simulation software (AVL Boost) are made [11]. The single zone turbulence model presented in [11] is extended to a two zone turbulence model. The aim of the two zone turbulence model is to slow down the flame propagation as the combustion approaches the end. In this way slowing down of the combustion is calculated by a physically based model unlike previous approach where a correlation base wall-combustion burning model was used. The two zone turbulence model is using a particular simplification which has not been documented before. Both (single and two zone) turbulence models are applied to the quasi-dimensional combustion model which divides the cylinder into a burned and an unburned zone.

During the development process, the results of the turbulence models were compared with the appropriate results of the turbulent quantities from the 3-D CFD calculations. By using this approach, the turbulence results were separated from the influence of combustion model. Once the turbulence quantities are matched, the combustion model was verified by comparing the results of combustion progress obtained by cycle-simulation and by 3-D CFD.

## Modeling of turbulence

### *Background*

Turbulent flow is usually described in terms of the steady mean value of velocity $\overline{u}_i$ and its fluctuating component $u_i'$ that oscillates around the mean value [1, 12]. Therefore, the instantaneous velocity $u_\mathrm{i}$ can be expressed as: $u_\mathrm{i}(t) = \overline{u}_\mathrm{i} + u_i'$. Besides velocity, all other quantities such as pressure and density vary in space and time and can also be expressed as a sum of the mean and the fluctuating part. This approach is often called the Reynolds decomposition [1].

The $k$-$\varepsilon$ turbulence model is the model that is most commonly used by researchers developing or applying multi dimensional codes in engineering problems. It includes two transport equations, one for the turbulent kinetic energy $k$ [$\mathrm{m^2s^{-2}}$] and the other for its dissipation rate $k$ [$\mathrm{m^2s^{-3}}$] [1, 8, 12]. The Reynolds averaged Navier-Stokes (RANS) equations are derived by the application of Reynolds decomposition and by neglecting fluctuations in density, pressure and viscous stress tensor. This paper is focused on the two-equation $k$-$\varepsilon$ turbulence model in which the Reynolds stress tensor is related to the gradients of velocity and eddy viscosity. The standard $k$-$\varepsilon$ turbulence model is based on the best understanding of the relevant processes that change the turbulent kinetic energy $k$ and its dissipation rate $\varepsilon$ [1, 13]. Differential equations of the standard $k$-$\varepsilon$ turbulence model are derived from RANS equations after the multiplication by the turbulence velocity $u'$ and averaging over time. They are employed in all CFD codes that use the $k$-$\varepsilon$ turbulence model.

### *Single zone k-ε turbulence model*

Production and dissipation of turbulent kinetic energy are always closely linked, which means that the dissipation rate is higher when the level of production of turbulent kinetic energy is high [1]. The production of turbulent kinetic energy is usually calculated by using the generally accepted Boussinesq approximation [1, 8, 14]. Assuming that there is equilibrium between the production and the dissipation of turbulent kinetic energy, standard differential equations of zero dimensional approach can be extended by including the diffusion term considered as a boundary flux between the burned and the unburned zone [8, 10]:

$$\frac{\mathrm{d}k}{\mathrm{d}t}=\frac{2}{3}\frac{k}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t}-\frac{2}{3}\frac{k}{\upsilon}\frac{\mathrm{d}\upsilon}{\mathrm{d}t}-\varepsilon \tag{1}$$

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}t}=\frac{4}{3}\frac{\varepsilon}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t}+\frac{5}{12}\frac{\varepsilon}{\upsilon}\frac{\mathrm{d}\upsilon}{\mathrm{d}t}-C_2\frac{\varepsilon^2}{k} \tag{2}$$

where $\nu$ [m$^2$s$^{-1}$] is the kinematic viscosity and $\rho$ [kgm$^{-3}$] is density of the cylinder mixture. If eqs. (1) and (2) are compared to the multi dimensional transport equations, one can notice that the zero dimensional model neglects the following: convective and diffusion change in turbulent kinetic energy and its dissipation rate, shear effects and the second order term in the dilatation effect of production.

The turbulence processes can be best understood by adopting the energy cascade phenomenon described in [15]. When the mass flows into the combustion chamber, the mean macroscopic velocity of the cylinder mixture increases as well as the mean kinetic energy. The mean kinetic energy is represented by large scale eddies that are unstable and therefore are decomposed into progressively smaller eddies. The turbulent kinetic energy is represented by small scale eddies that continuously become smaller and are finally dissipated into heat by the effect of viscous forces. This process is always unidirectional, which means that the turbulent kinetic energy can emerge only from the mean kinetic energy. During the exhaust, when the mass flows out of the cylinder, the mean and the turbulent kinetic energy decrease.

It is known from literature [6, 8-10] that the in-cylinder turbulent flow field can be considered to be homogeneous and isotropic during the late part of the compression stroke and near TDC. Since equations of the zero dimensional approach are derived assuming the homogenous and isotropic turbulent flow field, the turbulence model is applied only to the high pressure cycle. If the Reynolds number inside the combustion chamber is not large enough, the large scale eddies interact with the smaller ones and eqs. (1) and (2) are no longer valid. In order to apply eqs. (1) and (2) to the cases with different Reynolds numbers and to achieve results of the turbulent kinetic energy that would be comparable to the 3-D CFD results, an additional coefficient $C_{\mathrm{eps}}$ was added to eq. (2):

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}t}=C_{\mathrm{eps}}\left(\frac{4}{3}\frac{\varepsilon}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t}\right)+\frac{5}{12}\frac{\varepsilon}{\upsilon}\frac{\mathrm{d}\upsilon}{\mathrm{d}t}-C_2\frac{\varepsilon^2}{k} \tag{3}$$

Finally, eqs. (1) and (3) are used for the calculation of turbulence and they are implemented in the cycle-simulation software (AVL Boost). More details about the single zone turbulence model and its validation are presented in [11].

### *Two zone k-ε turbulence model*

As noted earlier, during combustion, the model of cycle-simulation software divides the cylinder mixture into two separated zones, burned and unburned. On the other hand, the turbulence model described above calculates only the mean turbulence kinetic energy and applies it to both zones. It is known from the combustion theory [16, 17] that physical properties of the unburned zone play the most important roles in the combustion process. The turbulent kinetic energy of the unburned zone causes convective deformation of the flame front, with additional transfer of momentum, heat, and mass. Therefore, in order to be able to predict the combustion progress better and physically more accurate, the turbulence kinetic energies of both zones should be calculated separately. This section describes the extension of the single zone turbulence model into a two zone turbulence model.

The previously defined single zone model [11] is able to calculate the mean turbulence kinetic energy of the cylinder mixture well. This fact was exploited in the development of the two zone model. Instead of setting the model that will calculate the changes in turbulence kinetic energy of the burned and of the unburned zone [6], the two zone model that is presented in this paper calculates the mean (total) turbulent kinetic energy and the turbulent kinetic energy of the unburned zone. The turbulence values of the burned zone can then be explicitly calculated by the mean values of the cylinder mixture and by the values obtained in the unburned zone. When the cylinder mixture is divided into the burned and the unburned zone, the conservation law of the total turbulent kinetic energy has to be satisfied. In accordance with this statement, several expressions can be written:

$$k_{\mathrm{tot}} = x_{\mathrm{B}} k_{\mathrm{BZ}} + (1 - x_{\mathrm{B}}) k_{\mathrm{UZ}} \tag{4}$$

$$P_{\mathrm{tot}} = x_{\mathrm{B}} P_{\mathrm{BZ}} + (1 - x_{\mathrm{B}}) P_{\mathrm{UZ}} \tag{5}$$

$$\varepsilon_{\mathrm{tot}} = x_{\mathrm{B}} \varepsilon_{\mathrm{BZ}} + (1 - x_{\mathrm{B}}) \varepsilon_{\mathrm{UZ}} \tag{6}$$

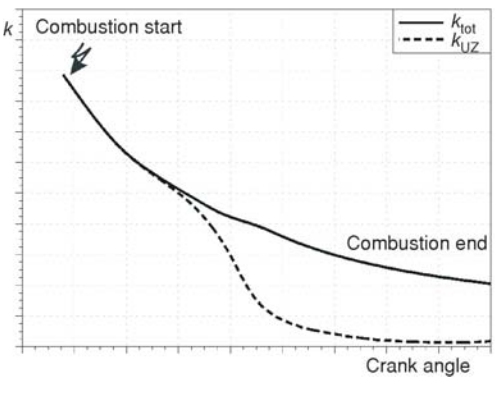


**Figure 1. Example of the turbulent kinetic energies from 3-D CFD during combustion**

where physical quantities with the index "tot" denote specific quantities related to the total cylinder mixture; "BZ" and "UZ" are related to the burned zone and unburned zone, respectively. Burned mass ratio $x_{\mathrm{B}}$ represents the ratio between the mass of the burned zone and the total in-cylinder mass. When the total and unburned zone turbulent kinetic energies are known, the turbulent kinetic energy of the burned zone can easily be computed from eq. (4). Results of the total turbulent kinetic energy and that of the unburned zone, calculated by 3-D CFD software, are shown qualitatively in fig. 1.

It can be seen that the turbulent kinetic energy of the unburned zone never exceeds the value of the total turbulent kinetic energy ($k_{\mathrm{UZ}} \leq k_{\mathrm{tot}}$). When one wants to obtain similar profiles by using the cycle-simulation model, the production-to-dissipation ratio of the specific zones has to be controlled. Since the two zone turbulence model strategy used here does not take into account the production and the dissipation rate of the burned zone, the full control between the production-to-dissipation ratio of total mixture and that of the unburned zone cannot be established.

The production of turbulent kinetic energy is almost always positive [14]. Negative production of turbulent kinetic energy means that the small scale eddies are merged together creating large scale eddies, which is in contradiction to the energy cascade phenomenon. The dissipation rate of turbulent kinetic energy is also always positive. Therefore, from eqs. (5) and (6), the following expressions can be written:

$$[P_{\rm tot} - (1 - x_{\rm B})P_{\rm UZ}] \geq 0 \tag{7}$$

$$[\varepsilon_{\rm tot} - (1 - x_{\rm B})\varepsilon_{\rm UZ}] \geq 0 \tag{8}$$

If conditions presented by eqs. (7) and (8) are not satisfied, corrections to the production and the dissipation rate of the unburned zone have to be made. The corrections are made by assuming that, in the case when the conditions presented by eqs. (7) and (8) are not satisfied, the production and the dissipation of the burned zone are 0. In that case, the correction to the production and the dissipation of the unburned zone is made in the following manner:

$$P_{\rm UZ} = \left(\frac{1}{1 - x_{\rm B}}\right) P_{\rm tot} \tag{9}$$

$$\varepsilon_{\rm UZ} = \left(\frac{1}{1 - x_{\rm B}}\right) \varepsilon_{\rm tot} \tag{10}$$

With the corrected production and dissipation, the change in turbulent kinetic energy and its dissipation rate of the unburned zone can be calculated by using a differential equation similar to that used in the single zone model:

$$\frac{{\rm d}k_{\rm UZ}}{{\rm d}t} = \frac{2}{3}\frac{k_{\rm UZ}}{\rho_{\rm UZ}}\frac{{\rm d}\rho_{\rm UZ}}{{\rm d}t} - \frac{2}{3}\frac{k_{\rm UZ}}{\upsilon_{\rm UZ}}\frac{{\rm d}\upsilon_{\rm UZ}}{{\rm d}t} - \varepsilon_{\rm UZ} \tag{11}$$

$$\frac{{\rm d}\varepsilon_{\rm UZ}}{{\rm d}t} = C_{\rm eps}^{\rm UZ}\left(\frac{4}{3}\frac{\varepsilon_{\rm UZ}}{\rho_{\rm UZ}}\frac{{\rm d}\rho_{\rm UZ}}{{\rm d}t}\right) + \frac{5}{12}\frac{\varepsilon_{\rm UZ}}{\upsilon_{\rm UZ}}\frac{{\rm d}\upsilon_{\rm UZ}}{{\rm d}t} - C_2\frac{\varepsilon_{\rm UZ}^2}{k_{\rm UZ}} \tag{12}$$

where $C_{\rm eps}^{\rm UZ}$ is the newly introduced user defined coefficient. Equations (11) and (12) are used together with eqs. (1) and (3), where the latter are used for the calculation of the change in the mean (total) cylinder turbulent kinetic energy and of its dissipation rate.

### Combustion modeling

Combustion process is a complex physical phenomenon which includes turbulence, chemical reactions and combustion chamber wall interaction. Studying and modeling turbulent combustion are important issues in the development and improvement of practical systems such as rockets, internal combustion engines, industrial burners, and furnaces. Numerical simulations of turbulent flames are a fast growing field because combustion is a complex phenomenon which is difficult to calculate by using analytical techniques [16]. There are a lot of combustion models available for multi dimensional calculations (flame-sheet models, flamelet models, eddy break-up model). An extended coherent flame model (ECFM) was used in the presented analysis in 3-D CFD calculations, while the fractal combustion model was used in the cycle-simulation software. Although the main equations of the fractal combustion model are already published before, the method of equations application is changed when two zone turbulence model is applied. Therefore, the model will be briefly described in the following section.

The fractal combustion model [4, 5] is one of the flamelet models where the flame front is considered as an infinitely thin and highly wrinkled area due to the effects of turbulent eddies of different length scales. During the gas exchange process and compression, calculations are carried out as a single zone model. After the occurrence of spark, the plasma formation and the flame kernel evolution take place. Kernel initiation process ends about 200 μs after the spark discharge, when the flame front reaches a radius of about 2 mm. During this period, the burning speed is very high and depends on the energy released by the ignition system. Due to the complexity of the kernel formation processes, the calculation of combustion starts at the end of the kernel initiation with a stable and spherically shaped smooth flame of 2 mm in radius. At this point, the cylinder mixture is divided into two separated zones, the burned and the unburned zone. The wrinkled flame front propagates through the unburned zone at the laminar flame speed $S_\mathrm{L}$ [4, 5]. If the single zone turbulence model is applied, the overall burning rate is calculated as a weighted mean of the two combustion rates:

$$\left(\frac{\mathrm{d}m_\mathrm{b}}{\mathrm{d}t}\right)_\mathrm{total} = (1-w_2)\left(\frac{\mathrm{d}m_\mathrm{b}}{\mathrm{d}t}\right)_\mathrm{fract} + w_2\left(\frac{\mathrm{d}m_\mathrm{b}}{\mathrm{d}t}\right)_\mathrm{wall\text{-}comb} \tag{13}$$

where $w_2$ is the weight function that is equal to 0 during the fully developed turbulent combustion, $(\mathrm{d}m_\mathrm{b}/\mathrm{d}t)_\mathrm{fract}$ – the fractal combustion rate, and $(\mathrm{d}m_\mathrm{b}/\mathrm{d}t)_\mathrm{wall\text{-}comb}$ – the wall combustion burning rate. When the two zone turbulence model is used, the last term of eq. (13) can be omitted and the overall burning rate is equal to the fractal combustion rate. The fractal combustion rate can be calculated by the turbulent flame surface area $A_\mathrm{T}$ and the laminar flame speed $S_\mathrm{L}$:

$$\left(\frac{\mathrm{d}m_\mathrm{b}}{\mathrm{d}t}\right)_\mathrm{fract} = \rho_\mathrm{u} A_\mathrm{T} S_\mathrm{L} \tag{14}$$

where $\rho_\mathrm{u}$ is the unburned zone density.

The turbulent flame surface area $A_\mathrm{T}$ is calculated according to the fractal theory [18]:

$$A_\mathrm{T} = A_\mathrm{L}\left(\frac{L_\mathrm{I}}{l_\mathrm{k}}\right)^{D_3-2} \tag{15}$$

where $A_\mathrm{L}$ is the laminar flame surface area and $L_\mathrm{I}$ and $l_\mathrm{k}$ are the maximum and the minimum length scales of turbulent eddies. The laminar flame surface area $A_\mathrm{L}$ is calculated as a fully smooth area of the sphere whose center is located in the spark plug position. The fractal dimension $D_3$ is a function of the laminar flame speed $S_\mathrm{L}$ and the turbulent intensity $u'$ [5, 19]:

$$D_3 = \frac{D_{3,\max} u' + D_{3,\min} S_\mathrm{L}}{u' + S_\mathrm{L}} \tag{16}$$

where $D_{3,\min}$ and $D_{3,\max}$ are the lower and the upper limit of the fractal dimension, respectively. Equation (16) shows that a higher value of turbulent kinetic energy increases the fractal dimension, which then increases the wrinkled turbulent flame surface area $A_\mathrm{T}$, eq. (15). The maximum integral length scale required for eq. (15) is calculated directly from the turbulent kinetic energy ($k$) and its dissipation rate ($\varepsilon$) [1]:

$$L_\mathrm{I} = \frac{\sqrt{k^3}}{\varepsilon} \tag{17}$$

Unlike the single zone turbulence model where the mean (total) cylinder values of $k_{tot}$ and $\varepsilon_{tot}$ are used, the two zone turbulence model uses the turbulent kinetic energy and the dissipation rate of the unburned zone ($k_{UZ}$ and $\varepsilon_{UZ}$).

The minimum length scale is calculated assuming the isotropic turbulence [20]:

$$l_k = \frac{L_I}{\sqrt[4]{\mathrm{Re}^3}} \tag{18}$$

where Re is the Reynolds number. In a two zone turbulence model, the Reynolds number is based on the quantities of the unburned zone.

This change in calculation of minimum and maximum integral length scale changes the calculated ratio used in eq. (15) which defines the turbulent flame surface. This finally has an impact on the calculation of combustion progress.

The ratios of maximum to minimum integral length scales during the combustion process are shown in fig. 2. The first profile (full line) is based on the mean (total) turbulent quantities that are calculated when the single zone $k$-$\varepsilon$ turbulence model is used. The second profile (dashed line) is the profile obtained when the unburned zone turbulent quantities are used, which is made possible when the two zone $k$-$\varepsilon$ turbulence model is applied. Since the turbulent kinetic energy and the volume of the unburned zone rapidly decrease during combustion, it is logical that the maximum length scale (characteristic for large scale eddies) decreases and that the ratio of integral length scales decreases. This behavior results in the fact that the turbulent flame surface at the late part of the combustion becomes very similar to the laminar one. Besides that, the fractal dimension also comes close to the minimum value as the combustion comes to an end because the turbulent intensity of the unburned zone at the late part of the combustion is very low. When turbulent quantities of the unburned zone are used in the calculation of combustion, the slowing down of the combustion process at the late stages is correctly predicted, which makes the wall-combustion part of the calculation unnecessary, eq. (13).

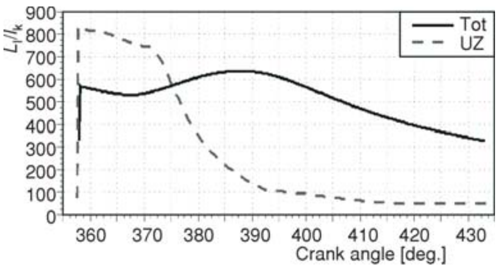


**Figure 2. Ratios of maximum of minimum integral length during combustion**

## Simulation results and discussion

The validation of the single and two zone turbulence models implemented in the cycle-simulation software was performed with respect to the 3-D CFD results of two single cylinder engine models. Part load and full load cases for low and high engine speeds were analyzed. Computational meshes of 3-D CFD models at TDC are shown in fig. 3. Unstructured moving meshes were used with a different number of computational cells. The cycle-simulation model which corresponds to both engines is shown on the right side of fig. 3. Different ge-

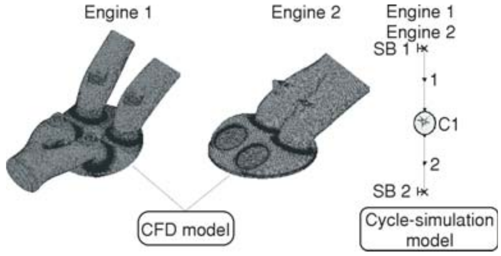


**Figure 3. Simulation models in the 3-D CFD and in the cycle-simulation model [11]**

ometries of the combustion chamber are defined by the specification of chamber geometry parameters such as bore, stroke, height of the combustion head, angles of the pentroof shape, ridge eccentricity, *etc*.

**Table 1. Specifications of single cylinder engine**

| | Engine 1 | Engine 2 |
|---|---|---|
| Displaced volume | 550 $cm^3$ | 400 $cm^3$ |
| Stroke | 95 mm | 81 mm |
| Bore | 86 mm | 79 mm |
| Connecting rod | 147 mm | 137 mm |
| Compression ratio | 11.1:1 | 11.1:1 |
| Number of valves | 4 | 4 |
| Exhaust valve open | 40° CA bBDC | 40° CA bBDC |
| Exhaust valve close | 10° CA aTDC | 20° CA aTDC |
| Inlet valve open | 25° CA bTDC | 5° CA bTDC |
| Inlet valve close | 50° CA aBDC | 55° CA aBDC |

The calculation model is comprised of the cylinder (C1), the intake and the exhaust pipes and the system boundaries (SB1 and SB2). In system boundaries, the specific boundary conditions (pressure, temperature, mixture composition), close to the intake and exhaust valves are defined. The main geometric parameters of the two different engines are specified in tab. 1. Validation was performed by simulating two operating points of each engine. Two different loads of Engine 1 at 2000 rpm and two different engine speeds at full load (wide open throttle – WOT) of Engine 2 were considered. Each operating point was simulated with the single and the two zone $k$-$\varepsilon$ turbulence model. Turbulence model coefficients that were used in the simulations are listed in tab. 2. The coefficient $C_{ign}$ represents the ignition formation multiplier which is used for tuning the ignition delay [21]. Since this coefficient linearly increases or decreases the time of the ignition delay, it has to be calibrated for each operating point. This is the main

**Table 2. Overview of the used constants and coefficients in the cycle-simulation software**

| | Engine 1 | | Engine 2 | |
|---|---|---|---|---|
| | Operating conditions | | | |
| | Case 1 | Case 2 | Case 1 | Case 2 |
| Engine speed | 2000 rpm | 2000 rpm | 1500 rpm | 5500 rpm |
| Engine load | 2.9 bar BMEP | WOT | WOT | WOT |
| Spark timing | 35° CA bTDC | 5° CA bTDC | 0° | 16° CA bTDC |
| A/F ratio | 14.5 | | | |
| Fuel type | Gasoline | | | |
| Mix. preparation | External | | | |
| | Single and two zone $k$-$\varepsilon$ parameters | | | |
| $C_2$ | 1.92 | | | |
| $C_{eps}$ | 2.35 | | | |
| $C_{eps}^{UZ}$ | 3.50 | | | |
| | Parameters of fractal combustion model | | | |
| $C_{ign}$ | 7.50 | 2.00 | 0.001 | 1.60 |
| $C\tau$ | 0.90 | | 0.50 | |
| $x_B$ at wall comb. start | 0.55 (1z); – (2z) | 0.45 (1z); – (2z) | 0.70 (1z); – (2z) | 0.50 (1z); – (2z) |
| $D_{3,max}$ | 2.45 (1z model); 2.52 (2z model) | | | |

disadvantage of the current combustion model and further improvements should include the definition of ignition delay based on certain physical phenomena. In order to calculate the development of the fully turbulent flame, *i. e.* the transition period from the laminar to turbulent flame, the following expression is used [22]:

$$\Delta t = 0.55 C_\tau \frac{L_I}{u'} \tag{19}$$

where $L_\mathrm{I}$ and $u'$ are the integral length scale and the turbulence intensity at the start of combustion, respectively.

The coefficient $C_\tau$ is the user-defined coefficient listed in tab. 2 and should be calibrated for certain engine configurations. The transition time calculated by eq. (19) is equal to the time required for the decay of the turbulent eddies at the start of combustion.

When the flame front reaches the cylinder walls, the combustion process is slowed down. The wall limits the gas expansion, constrains all flows, and cools the expanding gases. All of these factors change the fundamental behavior of combustion that is significantly different from that of a flame propagating freely across the chamber. The wall combustion burning rate, eq. (13), is applied when the specific ratio of burned mass is reached. It is defined by the user constant $x_\mathrm{B}$ listed in tab. 2. When the two zone *k*-$\varepsilon$ turbulence model is used, the unburned zone turbulence quantities (integral length scales, turbulence intensity) define the propagation of the flame across the chamber and the wall combustion burning mode is omitted. In this case the user-defined constant $x_\mathrm{B}$ is not necessary.

Various theories have been proposed [19, 21] for the upper limit of the fractal dimension ($D_{3,\max}$) in a premixed flame propagating through a flow field with a large Reynolds number. In this analysis, the upper limit of the fractal dimension is set to the uniform value $D_{3,\max} =$ $= 2.45$ when the single zone turbulence model is applied, and to the uniform value $\mathrm{D}_{3,\max} = 2.52$ in the case of two zone turbulence model. The values of $D_{3,\max}$ are the same in both engine geometries. Both turbulence model coefficients, $C_\mathrm{eps}$ and $C_\mathrm{eps}^\mathrm{UZ}$ are set to a single value for both engines in all conditions, giving very good agreement of the turbulent kinetic energies and the progress variables compared to 3-D CFD results.

The reference results for comparisons were obtained by 3-D CFD simulations. These simulations were performed as full cycle simulations including the intake and the exhaust stroke. The presented results of turbulent kinetic energies calculated by 3-D CFD code are mass averaged so that the values can be compared with the cycle-simulation results. Mass averaging is performed within the domain of interest, *i. e.* within the entire cylinder, the burned zone and the unburned zone. The separation of zones is defined on the basis of the value of progress variable within each computational cell.

Since transport eqs. (1) and (3) of the *k*-$\varepsilon$ turbulence model are not supposed to be applied during the gas exchange process, the calculation of turbulence within the cycle simulation is started at the intake valve closure (IVC). The initial value of the turbulent kinetic energy (at the IVC) in the cycle-simulation model is defined from the 3D-CFD result at the time that corresponds to the IVC event. On the other hand, the initial value of dissipation rate ($\varepsilon$) could not be defined in the same way. Since transport eqs. (1) and (3) are not the same as the ones in 3-D CFD, the same initial value of dissipation rate would give a different initial gradient of turbulent kinetic energy in a cycle-simulation model. Therefore, the initial value of dissipation rate is obtained from eq. (1), satisfying the condition that the gradient of turbulent kinetic energy is the same in 3-D CFD and in the cycle-simulation model at the IVC.

Two simulation runs of Engine 1 were performed at 2000 rpm with the part and the full load. Results of the total turbulent kinetic energies ($k_{tot}$) are shown in fig. 4. The prediction of the total turbulent kinetic energy obtained by cycle-simulation is in good agreement with 3-D CFD results. The shapes of the curves are correctly predicted, only the peak values are slightly under predicted in this engine configuration. Since the zero dimensional approach of turbulence model is based on the assumption of homogeneous and isotropic flow field, the under prediction of peak values can be explained by neglecting convective and diffusion effects [10]. The most interesting part of the process is the turbulent combustion phase since in this period the turbulence quantities influence the combustion. The starts of combustion marked with vertical dashed lines are presented in fig. 4. It can be observed that the total kinetic energies during combustion are predicted very well.

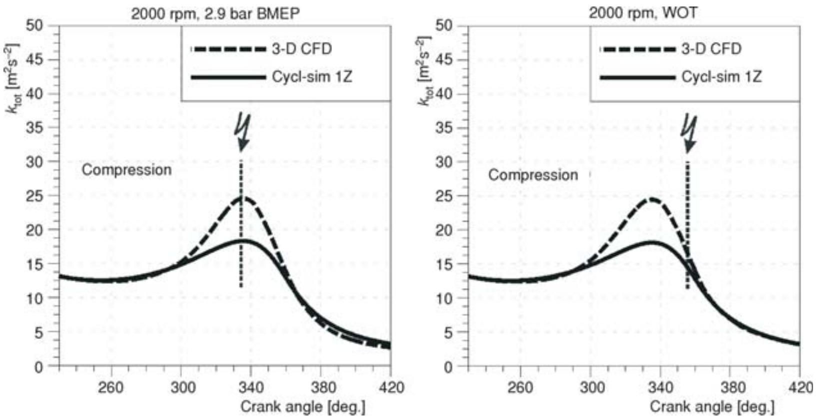


**Figure 4. Total turbulent kinetic energy; Engine 1 – Case 1 (left) and Case 2 (right)**

Figure 5 presents the level of the turbulent kinetic energies in the burned (BZ) and the unburned zone (UZ). The total kinetic energy of the two zone model is almost the same as in the single zone model since the equations are the same. The left boundaries of fig. 5 are the start of combustion which are marked with vertical dashed lines in fig. 4. During the early combustion phase, there is a difference in the prediction of $k$ in the BZ, but this zone is at that moment small

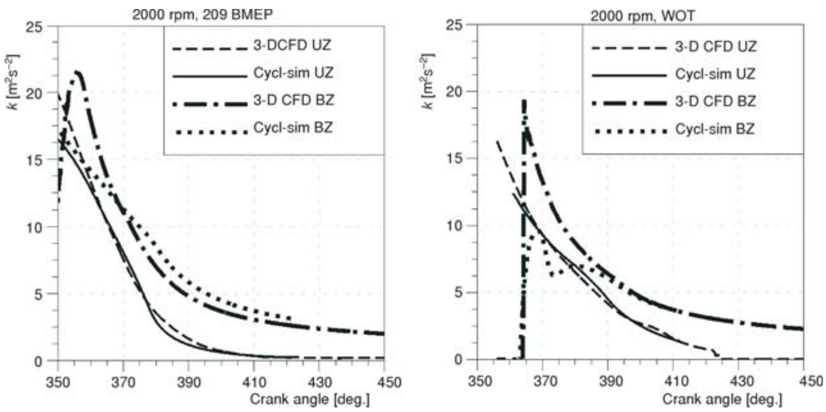


**Figure 5. Unburned and burned turbulent kinetic energy; Engine 1 – Case 1 (left) and Case 2 (right)**

and does not have a significant influence on the overall turbulence or on the combustion. Turbulent kinetic energy of the UZ which is used in the calculation of combustion is predicted very well.

The application of two zone $k$-$\varepsilon$ turbulence model shows a significant improvement to the cycle-simulation model in terms of prediction of the combustion process without the necessity for artificial wall combustion. This can be seen in fig. 6. Both calculations (1Z and 2Z) show a good comparison of the progress of combustion, but in the case of two zone model, the slowing down of combustion comes as a consequence of progress of turbulent kinetic energy in the UZ.

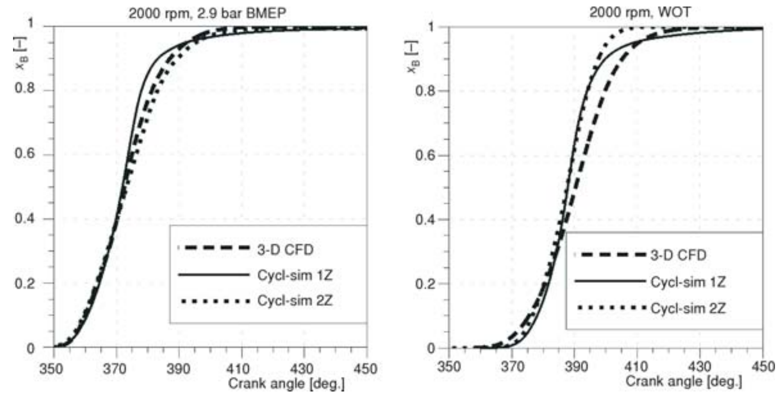


**Figure 6. Progress variable; Engine 1 – Case 1 (left) and Case 2 (right)**

In tab. 2 one can notice that most of turbulence coefficients are the same in both conditions, and in fact they are the same in both engine geometries. The ignition formation multiplier $C_{ign}$ is different in each case, and this has been noted earlier as a possible improvement to the model. In the case of single zone turbulence model, the wall combustion constant $x_B$ is different in each case, but when the two zone turbulence model is used there is no need to define this constant. The only coefficient that is changed in the two engine geometries, besides $C_{ign}$, is the coefficient $C_\tau$. The same results as the ones shown in figs. 4-6, but now for different engine geometry and conditions (Engine 2), are shown in figs. 7-9.

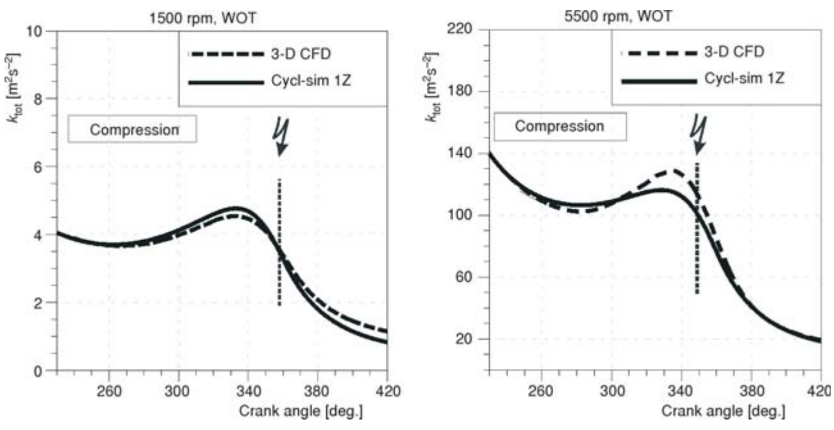


**Figure 7. Total turbulent kinetic energy; Engine 2 – Case 1 (left) and Case 2 (right)**

In the second engine geometry, the cases are characterized by different engine speeds at full load. The results from the second geometry show a better prediction of peak values of the turbulent kinetic energy that occur near TDC. The profile during combustion is also predicted well in these cases. Figure 8 again shows how levels of turbulent kinetic energies in BZ and UZ are different during combustion and that the two zone model can capture the profiles of both values during most of the combustion period. The mass burning rate represented by the progress variable is also predicted very well without using the wall combustion in the two zone model.

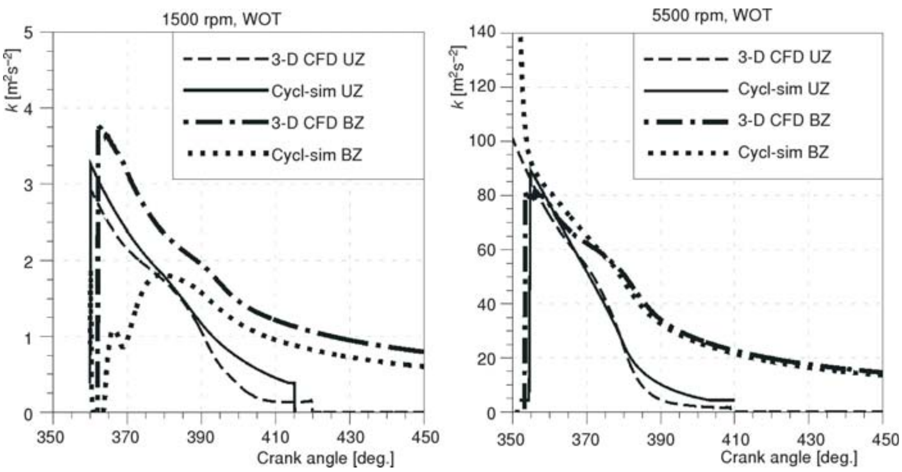


**Figure 8. Unburned and burned turbulent kinetic energy; Engine 2 – Case 1 (left) and Case 2 (right)**

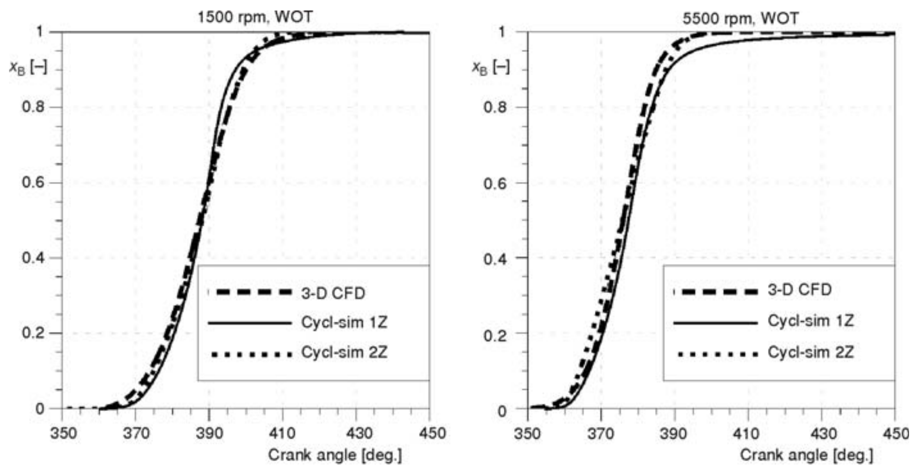


**Figure 9. Progress variable; Engine 2 – Case 1 (left) and Case 2 (right)**

Comparison of the results of engine 1 and 2 and their conditions show that the change in overall turbulence when engine load is changed is much smaller than the change that occurs when the engine speed is changed. A change in the engine speed from 1500 rpm to 5500 rpm has changed the total turbulence kinetic energy by almost two orders of magnitude. The turbulence model presented here has captured these differences although most of the differences are a consequence of changes during the intake process which is not modeled here. The influence of changes during the intake process is captured here by different initial conditions. Further improvement to the model could include modeling of the intake process which would make the calculation of cycle-simulation model independent on the initial conditions.

### Sensitivity analysis

The sensitivity analysis gives the information regarding the influence of some input parameters on the output results, particularly when the new coefficients are introduced in the model. The influence of the coefficient $C_{eps}$ on the overall turbulence level and on the combustion progress is demonstrated and described in detail in [11]. The sensitivity of two zone *k-ε* turbulence model to the value of new coefficient $C_{eps}^{UZ}$ is presented in fig. 10 where all other parameters were kept constant. A lower value of $C_{eps}^{UZ}$ coefficient decreases the dissipation rate of the UZ producing a higher turbulent kinetic energy of the same zone. On the other hand, by increasing $C_{eps}^{UZ}$ coefficient the turbulent kinetic energy of the UZ is slightly reduced as it is shown in fig. 10 (left). Since $C_{eps}^{UZ}$ coefficient does not have any influence on the total in-cylinder turbulence level, the results of this value are not shown here.

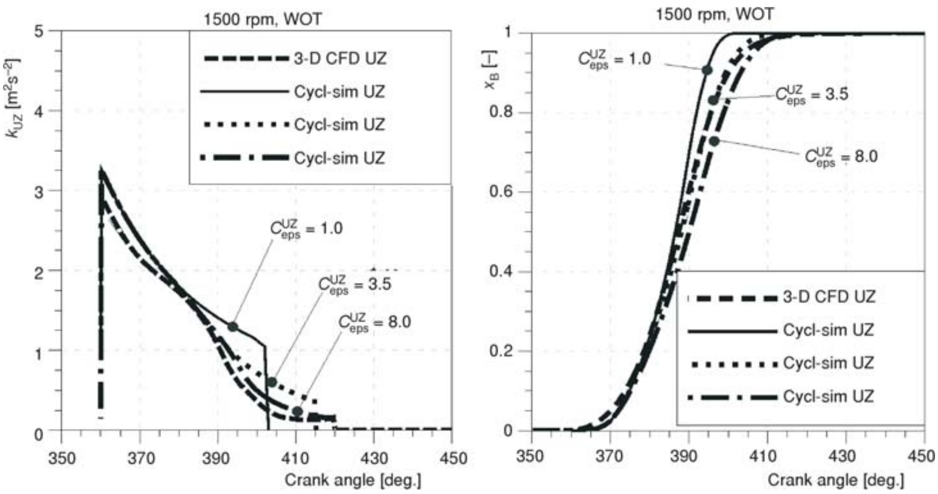


**Figure 10. Influence of coefficient $C_{eps}^{UZ}$ on the unburned zone turbulent kinetic energy (left) and on the combustion progress (right); Engine 2 – Case 1**

Influence of the $C_{eps}^{UZ}$ coefficient on the combustion process, shown in fig. 10 (right), is reasonable due to the dependence of combustion process on the UZ turbulence level. From the above figure it is evident that there are no significant changes during the early combustion phase (until ~30% of the cylinder mixture is burned). During the later part of the combustion, some differences can be observed. Lower value of $C_{eps}^{UZ}$ produces larger values of turbulence which then leads to faster combustion rates. But when these differences are compared to the differences obtained when $C_{eps}$ is changed (described in [11]), it can be concluded that the proposed *k-ε* turbulence model is weakly sensitive to the value of $C_{eps}^{UZ}$ coefficient. Therefore, more attention should be paid on the selection of the $C_{eps}$ coefficient when one wants to obtain a good prediction of turbulence quantities and combustion process.

## Conclusions

The extension of a single zone $k$-$\varepsilon$ turbulence model to a two zone $k$-$\varepsilon$ turbulence model for the zero dimensional approach applied in the cycle-simulation software has been presented. Since the isotropic and homogenous turbulent flow field is assumed, the implemented $k$-$\varepsilon$ turbulence model is applied only to the high pressure cycle, from the intake valve closure till the exhaust valve opening. In the development of the two zone model, a specific approach was taken. Instead of modeling the turbulent kinetic energy of the burned and the UZ, equations of the total turbulent kinetic energy and of the turbulent kinetic energy of the UZ are calculated. The turbulent kinetic energy of BZ is then explicitly defined from the total and the turbulent kinetic energy of the UZ. Since the turbulent quantities of the BZ do not have influence on the calculation procedure, the proposed simplified approach represents an effective, robust and low-computational-effort solution. Similarly to the single zone model when the $C_{\mathrm{eps}}$ coefficient is introduced to the dissipation rate equation, $C_{\mathrm{eps}}^{\mathrm{UZ}}$ coefficient is introduced in the equation for dissipation rate of the UZ, enabling the cycle-simulation model to be applied for both low and high Reynolds numbers.

The single and two zone $k$-$\varepsilon$ turbulence models were validated with the results from 3-D CFD calculations of two engine geometries with different loads and speeds. Comparisons of turbulent kinetic energies of different model domains (total, burned and unburned zone) show very good agreement. The turbulence model is able to predict the quantities and profiles of the mentioned values during compression, combustion, and expansion. The main disadvantage of the implemented turbulence model is the specification of initial conditions for the turbulent kinetic energy and its dissipation rate at the beginning of the high pressure cycle. In the presented model, the initial conditions are specified from the 3-D CFD results. Further work will include the extension of the turbulence modeling to the gas exchange process as well.

A combustion model that uses the calculated turbulence values was validated by comparing the results of progress variables calculated by the 3-D CFD and by the cycle-simulation software. These comparisons show very good agreement. When the single zone $k$-$\varepsilon$ turbulence model is used, the wall-combustion burning model has to be employed so that the late stages of combustion process can be correctly predicted. The application of two zone $k$-$\varepsilon$ turbulence model shows significant improvement in the prediction of combustion using only the fractal combustion model. The calculation of wall-combustion burning rate is in this case omitted because the flame propagation is defined by the turbulence of the UZ.

An approach in which the simplified modeling of SI combustion is supported by more complex and precise models (3-D CFD) is also presented in the paper. The process of modeling is in this case divided into the modeling of turbulence and the modeling of combustion which uses the obtained turbulence values. This approach enables cross-referencing of the results obtained by 3-D CFD and by cycle-simulation models. The sensitivity analysis performed within this work showed that the influence of the newly introduced $C_{\mathrm{eps}}^{\mathrm{UZ}}$ coefficient of two zone $k$-$\varepsilon$ turbulence model is low. If one wants to obtain a good prediction of turbulence quantities as well as combustion process, more attention should be paid on the selection of coefficient $\mathrm{C}_{\mathrm{eps}}$.

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The presented results were achieved during the project of implementation of the $k$-$\varepsilon$ turbulence model in the cycle-simulation software and during the project "Biofuels – the necessity for sustainable mobility in the Republic of Croatia".

## Nomenclature

$C_2$ – coefficient, [–]
$D_3$ – fractal dimension, [–]
$k_{tot}$ – total turbulent kinetic energy of the cylinder mixture, [$m^2s^{-2}$]
$k_{UZ}$ – turbulent kinetic energy of the unburned zone, [$m^2s^{-2}$]
$k_{BZ}$ – turbulent kinetic energy of the burned zone, [$m^2s^{-2}$]
$P_{tot}$ – total production of the turbulent kinetic energy, [$m^2s^{-3}$]
$P_{UZ}$ – production of the turbulent kinetic energy of unburned zone, [$m^2s^{-3}$]
$P_{BZ}$ – production of the turbulent kinetic energy of burned zone, [$m^2s^{-3}$]
$\Delta t$ – transition time from laminar to fully developed turbulent flame, [s]
$u'$ – turbulence intensity, [$ms^{-1}$]
$x_B$ – burned mass ratio (= $m_{BZ}/m$), [–]
$w_2$ – weight function, [–]

*Greek symbols*

$\varepsilon_{tot}$ – total dissipation of the turbulent kinetic energy, [$m^2s^{-3}$]
$\varepsilon_{UZ}$ – dissipation of the turbulent kinetic energy of unburned zone, [$m^2s^{-3}$]
$\varepsilon_{BZ}$ – dissipation of the turbulent kinetic energy of burned zone, [$m^2s^{-3}$]

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