

A Model for Prediction of Knock in the Cycle Simulation by Detail Characterization of Fuel and Temperature Stratification

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ABSTRACT

Development of SI engines to further increase engine efficiency is strongly affected by the occurrence of engine knock. Engine knock has been widely investigated over the years and the main promoting parameters have been identified as load (temperature and pressure), mixture composition, engine speed, characteristic of the fuel, combustion chamber design, and etc. In this paper a new model for predicting engine knock in 0-D environment is presented. The model is based on the well-known approach of using a Livengood and Wu knock integral. Ignition delay data that are supplied to the knock integral are for specific fuel calculated by detail chemical kinetics and are comprised of low temperature heat release ignition delay and high temperature heat release ignition delay. Next, the cycle to cycle variations of engine and temperature stratification of the end gas have to be taken into account. For temperature stratification a new model is developed which is based on the detail analysis of specific CFD results of several engines at different operating conditions. The validation of the knock prediction model was made by comparisons of the simulation results with the experimental data, for two different fuels (n-heptane and gasoline), showing promising ability of the model to predict the tendency of knocking. The results also showed that the cyclic variability of the knock occurrence and intensity in SI combustion is not only caused by the differences in pressure profile caused by cycle to cycle variations, but also by some other factors.

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INTRODUCTION

One of the important aspects of achieving high efficiency is increasing engine load. By increasing the engine load, the percentage of pumping and friction losses decreases and the brake efficiency increases, under assumption that other losses do not increase in the process. High load in SI engines can be obtained by boosting the intake air. Therefore the latest trend in development of advanced SI engines is production of highly boosted engines with small displacement. Once high boost is used the SI engine easily runs into knock conditions which have to be avoided. New research discoveries and technological advancements of engines are putting more and more devices which can be used for setting boundary conditions of an engine. Therefore a larger number of control variables can be used for optimizing engine operation, i.e. intake pressure, intake temperature, EGR, spark timing, and equivalence ratio. The optimization of engine operation with large design space is therefore very demanding in terms of human labor and time and the use of simulation in this process is desirable.

The simulation models of SI engines are continuously advancing with new models for physical effects that were previously not modeled. For use in optimization the model must run in reasonable time frame. For example in the last couple of years a lot of work has been done

on modeling of cycle to cycle variations (CCV) in SI engines [1, 2, 3, 4] which are very important in the process of knock occurrence. The developments of models that are capable of simulating CCV set the foundation for development of models in predicting engine knock on a cycle to cycle basis.

Engine knock is a mode of abnormal combustion which is not desirable because it can make severe damage to the engine. It has been identified that engine knock is caused by auto-ignition of the unburned end-gas whose temperature and pressure increases as a consequence of piston motion and the expansion of burned gas [5]. The main factors that influence the occurrence of knock are generally similar to the factors that influence the auto-ignition of a combustible mixture: pressure, temperature, equivalence ratio, mass fraction of combustion products, engine speed and fuel type. Thus, an accurate simulation model for predicting knock needs to model all the above mentioned factors in the region where knock occurs (end-gas) and has to model the auto-ignition behavior of the unburned mixture. This means that the ideal model would comprise a 3D model of the combustion chamber. In addition to computing the flame propagation, the model would include the detail chemical kinetics calculation in the unburned cells and the model would be run in a cycle to cycle calculation of CCV (e.g. LES or DNS). This type of simulation is not

practical for optimization and would require a huge amount of computation time. Therefore the simplifications of the models are made with specific assumptions.

Over the years, a number of numerical models for predicting knock have been developed with specific assumptions and simplifications. Many of the simplifications use the 0D approach where the cylinder charge is divided into a burned and unburned zone (two zone approach) each having different temperature and composition but both having the same pressure. In the two zone approach, the calculated temperature, pressure and composition of the unburned zone is used for prediction of auto-ignition of that zone. In some of the models, the calculation of auto-ignition is made by using detailed chemical kinetics [6, 7, 8, 9, 10, 11, 12]. Although this approach gives confidence in the modelling of behavior of the fuel, it is computationally still very demanding and not suitable for CCV. In order to simplify the chemistry of the fuel, reduced mechanisms have been made, e.g. Shell auto-ignition model [13], and used in models for prediction of engine knock [14, 15].

To speed up the calculation process, many models [4, 16, 17, 18, 19, 20, 21] computed the onset of auto-ignition based on the knock integral method introduced by Livengood and Wu [22]. The knock integral method requires information regarding the ignition delay of the unburned mixture during the entire combustion period. In most of the existing models, the ignition delay is calculated by a single or multiple equations that have Arrhenius rate form. These equations have been obtained by optimization of the rate coefficients and tuning them so that the computed ignition delay matches the ignition delay data obtained from measurement or detail chemical kinetics calculation. In some earlier papers, the equations for calculating ignition delay included only the influence of pressure and temperature, but recent models use equations that include the influences of equivalence ratio and EGR level as well, e.g. [4]. Besides equations that calculate ignition delay based on the specific conditions, some authors use look-up tables calculated by detail chemical kinetic. In [20] the knock integral is calculated by using ignition delay data taken from look-up tables that depend on temperature, pressure, equivalence ratio and mass fraction of combustion products. These look-up tables can be obtained by using a detail chemical kinetics prior to the 0-D calculation. In this way the error that comes as a consequence of non-correspondence of functional approximation of ignition delay data to the detail kinetics data is removed. The use of knock integral method significantly speeds up the calculation process and therefore this model can be used in multi cycle simulations that mimic CCV, e.g. [4, 20, 21].

In all of the publications listed above, except in the [20], the unburned zone is treated as homogeneous with uniform temperature and composition. In [21] the authors recognize that there is a thermal stratification of the end-gas and that the boundary layer near cylinder wall will be less prone to knock. In order to account for that the authors introduced a correction function to the knock integral. In [23] a stochastic reactor model that accounts for the thermal stratification on the statistical basis is used in an analysis of knock initiation. It has been concluded that in order to reconstruct the knock occurrence in the simulation, an initial reactor temperature distribution, with respect to the CFD simulation has to be included. In [4] the authors have

used a scaling factor on the correlation for calculation of ignition delay, although the correlation is obtained by a kinetic fit of the correlation to the detail kinetics results. The scaling of the correlation is made by comparison of experiment and simulation data. This scaling modifies the original ignition delay correlation so that the model is able to predict the occurrence of engine knock although all the effects, e.g. temperature stratification, are not taken into account. In [20] a CFD analysis of the end-gas was performed on the natural gas engine. It was found that a significant thermal stratification of the end-gas exists and that the thermal stratification should be included in the model that predicts knock. The conclusion that thermal stratification should be included in the model for predicting knock was also tested by running simulations of couple of cycles with heavy knock. In these simulations the detail chemical kinetics calculation is put on the unburned zone. It was found that the average conditions of the unburned zone were not sufficient to produce occurrence of auto-ignition. The results of these simulations were not shown in [20], but the following results justified the use of thermal stratification.

In [20] a novel approach in predicting knock based on multiple subzones of the unburned zone was introduced. The subzones were used to account for the thermal stratification in the unburned mixture and the model of thermal stratification was based on the statistical analysis of 3D - CFD results of the engine under consideration. Besides thermal stratification the model included the method of replicating CCV from experiment, while the occurrence of knock is predicted by a knock integral method that used look-up tables obtained by detailed chemical kinetic calculation using GRI 3.0 mechanism [24]. The results showed that although the approach did not give the exact correspondence of knock results in each individual cycle, on average basis the results showed promising ability to predict knock.

In [20] the model was validated against experimental results from engine fuelled by natural gas that does not show low temperature heat release (LTHR). Also, the model required a lot of input data, especially for temperature distribution, which had to be obtained from CFD model of the engine. In this paper a further advancement of the model approach shown in [20] is made which enables the use of the model with fuels that show LTHR behavior. The second advancement is made on the side of the temperature stratification calculation where the model is parameterized based on the 3D-CFD results from several engines and conditions, and now requires much less input data. The model was validated with the experimental results from two different fuels, n-heptane and gasoline, at several different engine conditions and compression ratios.

MODELING OF PREDICTION OF KNOCK

The work presented in this paper assumes that quasi-dimensional model of SI combustion, i.e. two zone fractal combustion model, will be able to correctly predict temperature and pressure of both burned and unburned zone on the cycle to cycle basis, as described in some earlier papers [1, 2]. With this assumption the task of the knock model is to predict whether at certain conditions engine knock occurs, what is the timing of knock and what is the intensity of that knock. Based on the presented scope of this paper the model for prediction of knock should have the following main features:

- The model must be fast so that a large number of cycles can be calculated in reasonable time.
- The model has to calculate temperature stratification of the unburned zone.
- The model has to calculate some value of knock intensity for each individual cycle.

In order to satisfy the above mentioned criteria and to calculate all the required results the knock prediction model has three specific sub-models: auto ignition sub-model, temperature stratification sub-model and knock intensity sub-model.

Auto-Ignition Sub-Model

The task of the auto-ignition sub-model is to predict the instant at which a certain part of the cylinder charge auto-ignites. Since the model takes into account the temperature stratification of the unburned zone, by dividing the unburned zone into several sub-zones, the prediction of auto-ignition will take place for each sub-zone. Because the model has to be fast, the calculation of detail kinetics is not an option and therefore the knock integral method is employed. In this method the knock integral (KI) is calculated for specific part of the cylinder charge, e.g. one representative unburned zone or multiple unburned zone sub-zones:

$$KI_i = \int_{t_{soc}}^t \frac{dt}{\tau_{d,i}} \quad (1)$$

where: τ_d [s] = ignition delay; i = index of area for which KI is calculated, e.g. unburned zone sub-zones; t_{soc} [s] = time of start of combustion; t [s] = instantaneous time.

The ignition delay that is required for the calculation of Eq. (1) is taken from look-up tables that depend on four different factors: pressure (p), temperature (T), equivalence ratio (ϕ) and mass fraction of combustion products (CP). The auto-ignition of the charge occurs when the value of the knock integral reaches a predefined threshold value (TR) which is usually set to 1. In this work the threshold value was set to $TR=0.95$ because that value gave the best correspondence of auto-ignition prediction obtained by specific detail chemical kinetics calculations and calculations that predicted auto-ignition by knock integral.

Ignition delay data represents the period of time for a charge at predefined pressure and temperature to reach auto-ignition. Ignition delay times can be measured by rapid compression machine or shock tube, but in this case the ignition delay data were calculated by using detail chemical kinetics calculation of constant volume reactor. The method of calculation and extraction of data is described in [25]. Figure 1 shows a typical profile of the temperature (T) obtained from the fuel that exhibit low temperature heat release in the conditions where this type of heat release occurs. Usually the first increase of T is discarded and only the position of main auto-ignition is recorded as τ_d . But, since low temperature heat release (LTHR) does occur in some fuels and can significantly influence the change of pressure and temperature before the main auto-ignition (high temperature heat

release HTHR) in this work both ignition delays are tabulated ($\tau_{d,LTHR}$, $\tau_{d,HTHR}$). Additionally the ratio of energy released during LTHR to overall energy released during entire combustion (r_{LTHR}) is also tabulated.

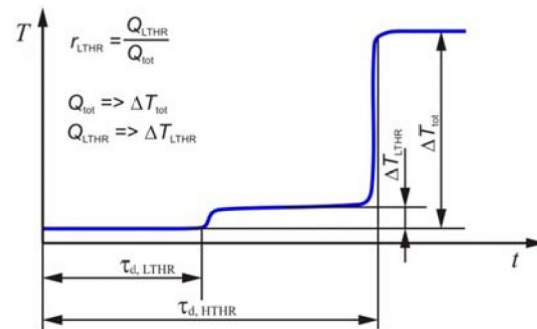


Figure 1. Profile of temperature or pressure obtained from constant volume reactor calculation for specific initial pressure, temperature, equivalence ratio and mass fraction of CP.

In order to include the influence of LTHR on the enhancement of auto-ignition and knock, and taking into account that tabulation described above saves data for ignition delay of LTHR and HTHR, two knock integrals are calculated for each zone or sub-zone simultaneously. One knock integral is calculated for LTHR and uses $\tau_{d,LTHR}$ in Eq. (1) while the second knock integral is calculated for HTHR and uses $\tau_{d,HTHR}$. Based on the values of these two knock integrals a decision of the type of auto-ignition in zone or sub-zone is made. While both knock integrals are lower than TR it is assumed that there is no heat release. If $KI_{LTHR} \geq TR$ and $KI_{HTHR} < TR$ it is assumed that LTHR occurs in that zone or sub-zone, while if $KI_{HTHR} > TR$ the HTHR will be triggered for that zone or sub-zone regardless of the value of KI_{LTHR} . Depending on the type of the auto-ignition the specific function for calculating the rate of heat release from that auto-ignition will be used. That will be described later in “Pressure and temperature calculation” section. By employing the proposed strategy the effects of the LTHR from each zone or sub-zone, in fuels that exhibit LTHR, on the overall knocking event are accounted for.

Temperature Stratification Sub-Model

The temperature stratification sub-model has to enable the implementation of non-uniform temperature distribution into the calculation of prediction of knock. Temperature stratification is modeled by dividing the unburned zone into arbitrary (N_{zn}) number of sub-zones, with equal mass, as presented in Figure 2. The mean unburned zone temperature is calculated by the standard quasi dimensional model of SI combustion, and in each step distributed into temperatures of defined number of sub-zones. For each sub-zone, based on the conditions in the sub-zone, knock integrals for LTHR and HTHR are calculated (Figure 2) and depending on the values of these knock integrals the decision regarding the occurrence of knock is made.

The distribution of temperatures in the subzones is modeled by a presumed shape of distribution which is based on the knowledge obtained from a number of 3D-CFD runs of different engine conditions. In this analysis the 3D-CFD calculations

of 4 different engines and 15 operating points were made with specific analysis of the results that enabled the development of the temperature distribution model. The 3D-CFD models are based on different engines that represent modern SI engine design, while the operating conditions are for each engine set so that the high and low engine speed condition at full load and at least one part load condition is covered.

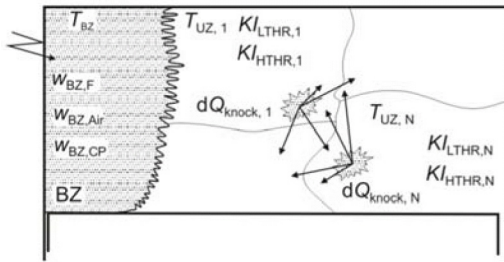


Figure 2. Dividing the unburned zone into sub-zones.

The 3D-CFD calculations were made in the AVL Fire program with unstructured moving meshes that had different number of computational cells at top and bottom dead center (for one engine the number of cells at TDC was 66168 and at BDC was 1226248; the other engines had similar structures). The entire cylinder domain was simulated and therefore no cyclic boundary conditions were used. The simulations were performed as RANS simulations with the standard k - ϵ turbulence model and the Three Zone-Extended Coherent Flame Model (3Z-ECFM) for turbulent flame propagation. Wall heat is calculated by a standard wall heat model in AVL Fire, which is based on the Jayatilke model.

After simulation, post-processing of the results was made to deduce profiles of temperature distribution in the unburned zone for each case at each crank angle. The process of post-processing of the results first selected the cells within the unburned zone. The cells were marked as unburned zone cells if the progress variable within the cell was lower than 0.1 and if the progress variable was higher than 0.1 the cell was counted as burned zone cell. The relatively low value of progress variable threshold is chosen so that only cells that do not have significant heat released from combustion are counted as the unburned zone cells. If a higher value of progress variable threshold is taken than some cells have unreasonably high temperatures for unburned zone conditions. After dividing the computational domain into burned and unburned zone the unburned zone part was subdivided into groups based on temperature. The temperature window for grouping of cells was 10 K and after that the mass fractions of groups were calculated. The output of the procedure is the mass fraction vs temperature plot of the unburned zone for each crank angle position and each operating point, as shown in Figures 3 and 4. Figure 3 shows the mass fraction vs temperature profile at start of combustion while Figure 4 shows the profile of the same operating point 30°CA later, i.e. at one point during combustion when mass fraction burned $MFB=0.64$. For each operating point and crank angle calculated by 3D-CFD the unburned zone has a maximum value of temperature and a minimum value of temperature. These two values define a temperature range of all the cells of the unburned zone at that operating point and crank angle.

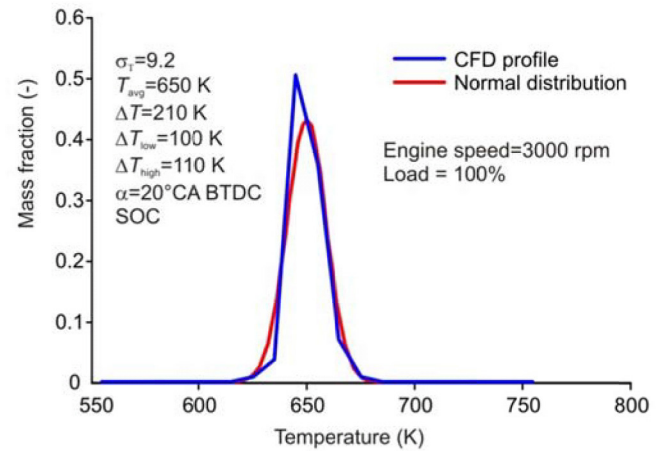


Figure 3. Mass fraction vs temperature profile of the unburned zone at start of combustion obtained by 3D-CFD calculation and the profile of normal distribution defined by the 3D-CFD results.

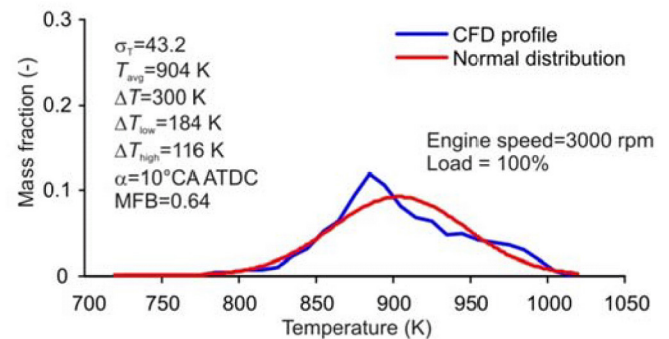


Figure 4. Mass fraction vs temperature profile of the unburned zone at the point during combustion obtained by 3D-CFD calculation and the profile of normal distribution defined by the 3D-CFD results.

The 3D-CFD results of mass fraction vs temperature are statistically analyzed and from that the average temperature of the unburned zone and the standard deviation of temperature for each crank angle and operating point were calculated. The values of these measures are also shown on the plots in Figures 3 and 4. In addition, on Figures 3 and 4 the profiles of normal distribution function, that were calculated by using the average value of temperature and the standard deviation obtained by statistical analysis of 3D-CFD results, are shown. It can be noticed that normal distribution function captures well the profile of temperature from 3D-CFD, and therefore could be used for calculating the temperature distribution. However, the normal distribution function is unbounded, which, if used in such form, could lead to unrealistic values of temperature on both ends, depending on the number of sub-zones. Therefore, instead of using the standard normal distribution function the sub-zone temperatures are calculated by clipped normal distribution. The procedure for the calculation of temperatures by using a clipped normal distribution is shown in Figure 5. In the example shown in Figure 5 the average temperature is 900 K, the temperature span is ± 126 K, standard deviation of temperature is 45 K and number of zones is 10. The y-axis in Figure 5 is probability of the temperature which is set to be proportional to mass fraction. The left and right ends of the normal distribution curve are cut at the boundary values obtained by adding (or subtracting)

temperature span value to the mean value. The area beneath the curve has to be equal to 1 and therefore after cutting the ends the curve is normalized so that this requirement is achieved.

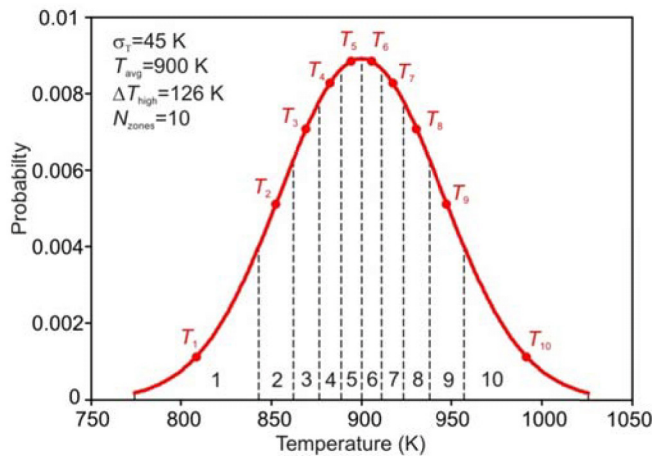


Figure 5. Calculating temperature by assumed temperature distribution

To calculate the mean temperatures of sub-zones the temperature spans of each sub-zone have to be defined. It is assumed that sub-zones have equal mass which means that the area beneath the curve for each temperature span that represents specific sub-zone has to be equal. In Figure 5 this boundaries of the sub-zones are marked by dashed vertical lines. It can be observed that the temperature spans of the hottest and coldest sub-zones are wider than the sub-zones around the mean value. Once the temperature boundaries of each sub-zone are defined the average value for each sub-zone is calculated by taking into account the mass fraction at each temperature position, which is assumed to be proportional to probability. The calculated average temperatures of the sub-zones are shown as dots on the profile curve. As can be noticed from a description of the procedure, the calculation of temperatures of the sub-zones require: average temperature, temperature difference between maximum (or minimum) temperature and the average temperature, and standard deviation of temperature profile. The average temperature in the simulation will be calculated by applied two zone model which means that models for standard deviation and temperature difference have to be made.

Further analysis of CFD results has been conducted to study how the temperature difference among the unburned zone and the standard deviation of temperature evolve during combustion. For each crank angle, we define ΔT_{high} as the difference between the maximum temperature and the average temperature. Similarly, ΔT_{low} is the difference between the average temperature and the minimum temperature. It has been observed that in each case there is a difference between ΔT_{high} and ΔT_{low} (see Figures 3 and 4), while in clipped normal distribution the temperature difference is symmetrical ($\Delta T_{high} = \Delta T_{low}$; Figure 5). Since knock will be initiated on the hot side of the unburned zone, the distribution of ΔT_{high} is more critical; therefore the distribution of ΔT_{high} is further analyzed. It has also been noticed that the absolute value of temperature difference changes

during combustion, but that during most of the combustion it can be correlated to average temperature. Therefore in Figure 6a the relative temperature difference, which is the ratio of temperature difference ΔT_{high} and average temperature T_{avg} , is shown as a function of mass fraction burned. It can be seen that the relative temperature difference has a very small average change during most of the combustion with sharp decrease at the end of combustion. The result shown in Figure 6a is the result of a single engine and operating point (the same as in figures 3 and 4), but the analysis of all other operating points and engines gave the same conclusion. The only difference between the cases is the approximate level of relative temperature difference during large part of combustion, which is in the case shown in Figure 6a around 0.15. Based on this the correlation function for relative temperature difference is defined as:

$$\frac{\Delta T_{high}}{T_{avg}} = a \left(1 - \frac{1}{100 \cdot (1 - MFB) + 1} \right) \quad (2)$$

In Eq. (2) the constant a is used to set the base level of relative temperature difference. The functional approximations of relative temperature difference with two different values of constant a (0.14 and 0.16) are also shown in Figure 6a. It can be noticed that by setting the appropriate parameter a , the proposed function approximates the 3D-CFD data well. The setting of parameter a will be discussed later.

The second value that has to be given to the calculation of sub-zone temperatures is standard deviation of T (σ_T). The standard deviation changes the value during combustion (as can be seen in Figures 3 and 4). The profile of change of standard deviation during combustion for a single engine and operating point is shown in Figure 6b. The profiles obtained on different engines and operating points showed similar pattern but with different maximum values ($\sigma_{T,max}$). Therefore in Figure 7 the normalized standard deviation of T obtained by statistical analysis of CFD results is shown. Normalized standard deviation of T is obtained by dividing the standard deviation of T for specific point during combustion with the maximum value of that operating point of the engine. In Figure 7 all the results from 4 different engines and all operating points are shown. The results are grouped into two groups: full load and part load cases. As can be seen the trend is similar but the part load cases seem to have linear increase of normalized σ_T with increase of mass fraction burned, while the full load cases follow slightly different pattern. Since knock is expected at high load cases only the full load cases are used in creation of approximation function. The profile of approximating function is also shown in Figure 7.

The approximating function shown in Figure 7 is used for the calculation of instantaneous value of σ_T , but only with defined maximum value ($\sigma_{T,max}$). The maximum value $\sigma_{T,max}$ is in this model supplied by the user of the model and can be used to tune the model with respect to 3D-CFD or experimental results.