

A RANS-Based CFD Model to Predict the Statistical Occurrence of Knock in Spark-Ignition Engines

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ABSTRACT

Engine knock is emerging as the main limiting factor for modern spark-ignition (SI) engines, facing increasing thermal loads and seeking demanding efficiency targets. To fulfill these requirements, the engine operating point must be moved as close as possible to the onset of abnormal combustion events. The turbulent regime characterizing in-cylinder flows and SI combustion leads to serious fluctuations between consecutive engine cycles. This forces the engine designer to further distance the target condition from its theoretical optimum, in order to prevent abnormal combustion to severely damage the engine components just because of few individual heavy-knocking cycles.

A RANS-based model is presented in this study, which is able to predict not only the ensemble average knock occurrence but also a knock probability. This improves the knock tendency characterization, since the mean knock onset alone is a poorly meaningful indication in a stochastic event such as engine knock. The model is based on a look-up table approach from detailed chemistry, coupled with the transport of the variance of both mixture fraction and enthalpy. These perturbations around the ensemble average value are originated by the turbulent time scale. A multivariate cell-based Gaussian-PDF model is proposed for the unburnt mixture, resulting in a statistical distribution for the in-cell reaction rate. An average knock precursor and its variance are independently calculated and transported, and the earliest knock probability is always preceding the ensemble average knock onset, as confirmed by the experimental evidence. This allows to identify not only the regions where the average knock first occurs, but also where the first knock probability is more likely to be encountered.

The application of the model to a RANS simulation of a modern turbocharged direct injection (DI) SI engine is presented and a small percentage of knocking cycles is predicted by the model although the average behavior is knock-free, in agreement with the experiments. The estimate of the knocking probability improves the consolidated "average knock" RANS analysis and gives an indication of the statistical knock tendency of the engine.

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INTRODUCTION

In the recent years, several established approaches to the numerical prediction of average engine knock were successfully developed in order to meet the requests derived from the SI engine trends. These demand thermal efficiency and specific output power to be raised to unprecedented levels, in order to reduce pollutant emissions and to simultaneously preserve the desired target performance.

Engine knock is the harmful consequence of the self-ignition of a portion of unburnt mixture before it is consumed by the main propagating flame front, and its occurrence is promoted by the mentioned strategies, as outlined in [1]. Given the need to operate as close as possible to the theoretical optimum of the regular combustion range, the occurrence of engine knock is a possibility that is always to be accounted for when the operating condition is

experimentally calibrated. To this aim, in-cylinder pressure is monitored in order to observe the random existence of knocking events. This is assessed by the definition of knock indices, such as the commonly adopted MAPO (Maximum Amplitude of Pressure Oscillations) or IMPO (Integral Modulus of Pressure Oscillations), as well as other indicators like the DKI (Dimensionless Knock Indicator) or the time-derivative of the in-cylinder pressure trace. Irrespectively of the chosen indicator, an arbitrary threshold value is always present to discern between a soft and acceptable knock intensity and a heavy and damaging knock level.

All the mentioned aspects motivate why a significant research effort was paid to knock prediction in the recent years. Remarkable examples of CFD models for average knock prediction are available in [2, 3], and the comparison against experiments assessed their accuracy in predicting the mean knock onset.

However, the ensemble average approach of RANS simulations when applied to knock modelling is intrinsically unable to reproduce the stochastic nature of knock, and this is becoming a critical factor for this type of analyses. This is due to the dramatic impact that cycle-to-cycle variability (CCV) has on all the in-cylinder physical processes, such as fuel-air mixing, combustion initiation and turbulent burn rate. Since engine knock depends on all the preceding processes, it is itself a typically stochastic and cycle-dependent phenomenon whose prediction is therefore extremely complex. The most rigorous approach to this analysis is the use of the Large-Eddy Simulation technique, which allows to simulate the large-scale portion of the unsteady engine flows. Although this kind of analysis represents a demanding study, several promising studies of this kind were presented in the recent years, such as the works by Robert et al. [4, 5].

Large-Eddy Simulation was used to predict knock occurrence in a turbocharged GDI unit by the authors in previous studies [6, 7, 8], and the cycle-dependent knock-signature well correlated with the outcomes from the experimental test-bench for both Knock-Limited Spark Advance (KLSA) and for a knocking regime with an advanced spark-timing.

Despite the mentioned recent application of the LES technique for engine CCV analysis, it still represents level of investigation which can be difficult to adopt at a design stage given the mentioned challenging computational cost. For this reason an alternative approach to model the random occurrence of knock was proposed by Linse et al. [9], which was based on a Probability Density Function (PDF) to account for a reconstructed knock distribution also in a RANS framework.

In this paper a RANS-based knock model based on a similar concept is proposed. The model accounts for the independent transport of an average knock precursor and of its variance, the combination of which gives an enhanced information not only regarding the average knock prediction but also estimating a distribution of knocking events around the mean one. Differently from the model presented in [9], a definition for a probability of knocking cycles is proposed based on the same statistical ground derived from the model equations.

In the next section a knock model based on cell-average values and detailed chemistry tabulation is presented as the representative of a family of models where the focus is put on the accuracy of the local reaction rate: to this aim a tabulation of detailed chemistry results is adopted, while average values for the local physical conditions are considered. Then, a statistically-grounded version of the same tabulated model is presented, and the turbulence-chemistry interaction is accounted for by considering transport equations for the local perturbation of the thermal and mixing status. Since the predicted fluctuations come from model equations, no artificial variation of flow variables is introduced. These are used to reconstruct a presumed distribution of reaction rates present in the fluid cell. Finally, the derivation of the mean knock precursor and of its variance are presented in details. The model is applied to a currently produced GDI engine, and the knock prediction given by the two numerical models is compared to the experimental results both in terms of average phasing and of frequency of individual

knocking events. A criterion is proposed to correlate the results from the PDF-based knock model with the number of knocking cycles, and the potentiality and the limitations of the presented model are critically presented and discussed.

KNOCK MODELLING

Cell-Average Knock Model

The first method is based on the interpolation of the AI delay considering the cell-wise Favre-averaged physical conditions, i.e. the input vector φ for the AI delay considers the cell-average values of absolute pressure, unburnt temperature, equivalence ratio and residuals mass fraction (Eq. 1).

$$\varphi = \varphi(\bar{p}, \bar{T}_u, \bar{\Phi}, \bar{Y}_{EGR}) \quad (1)$$

The φ vector lists the independent variables that govern a multiple interpolation technique whose result is the AI delay time $\bar{\tau}$. In this study the Andrae et al. [10] Toluene Reference Fuel (TRF) mechanism is adopted to generate a detailed look-up table of AI delays.

This approach constitutes a comprehensive model to consider the local physical conditions, since the AI delay time $\bar{\tau}$ fully describes the cell-wise reaction rate $\bar{\omega}$ through Eq. 2:

$$\bar{\omega} = \frac{1}{\bar{\tau}} \quad (2)$$

Once the local reaction rate $\bar{\omega}$ is available, a knock precursor concentration I is time-integrated following the Livengood-Wu knock integral function [11] and reported in Eq. 3.

$$I = \int_{t_0}^t \bar{\omega} dt = \int_{t_0}^t \frac{1}{\bar{\tau}} dt \quad (3)$$

The expression in Eq. 3 is the source term representing the progress of chemical pathway towards the possible autoignition. Finally the knock precursor I transport is modelled through a dedicated balance equation (Eq. 4) where the mentioned source term is accounted for.

$$\frac{\partial \bar{\rho} I}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{v} I) = \nabla \cdot (\bar{\rho} (D + D_T) \nabla I) + \bar{\rho} \bar{\omega} \quad (4)$$

When the local I value reaches unity in a portion of the unburnt fluid region, knock is locally triggered and time t identifies the knock timing. In Eq. 3 t_0 represents a conventional initial time after which the mixture reaction rate is relevant and its inverse (i.e. the cell-averaged $\frac{1}{\bar{\tau}}$ term) has to be time-integrated; in the present study this timing is assumed to be at the half of the compression stroke.

The limitation of this method is identified in the use of cell-based Favre-averaged values for the input variables contained in the φ vector. This implies that for a generic fluid cell a perfectly uniform value of pressure, unburnt temperature, equivalence ratio and residuals mass fraction is assumed. The consequence of such a

treatment is that for the sake of AI delay calculation every fluid cell is considered as a laminar well-stirred reactor. Even in a RANS framework, ensemble average turbulence may affect the local thermal and mixing state, as it will be shown in more detail in the next section. This can potentially induce variations in the reactivity of the unburnt charge and it is totally neglected in the Cell-Average knock method, hence the model can only provide information regarding the average knock onset. This aspect constitutes the main motivation for the PDF-Knock model presented in the next section.

PDF-Knock Model

The proposed method is an extension of the previously described approach to integrate the cell-wise reaction rate. The major difference with respect to the Cell-Average model is the statistical reconstruction of the physical states which are simultaneously present in the same fluid cell. Their dispersion around the mean value is originated by the local turbulence intensity, leading to two independent knock precursors and to a more statistically-based knock prediction than the Cell-Average knock model. In the following section the model equations are explained in detail.

PDF-Knock Model Equations

Two additional transport equations are solved in the PDF-Knock Method to independently account for local values of the sensible enthalpy and mixture fraction variance, h' and Z' respectively. They are reported in [Eq. 5](#) and [6](#).

$$\frac{\partial \bar{\rho} h'}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{v} h') = \nabla \cdot (\bar{\rho} (D + D_T) \nabla h') + 2\bar{\rho} D_T |\nabla h'|^2 + \bar{\rho} \frac{h'}{\tau_{Z(Re_{l_0})}} \quad (5)$$

$$\frac{\partial \bar{\rho} Z'}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{v} Z') = \nabla \cdot (\bar{\rho} (D + D_T) \nabla Z') + 2\bar{\rho} D_T |\nabla Z'|^2 + \bar{\rho} \frac{Z'}{\tau_{Z(Re_{l_0})}} \quad (6)$$

The difference from the standard transport equations used for enthalpy h and mixture fraction Z is condensed in the source terms, $\bar{\rho} \frac{h'}{\tau_{Z(Re_{l_0})}}$ and $\bar{\rho} \frac{Z'}{\tau_{Z(Re_{l_0})}}$ respectively. They are a function of the local turbulent Reynolds number Re_{ρ} , from which a turbulent relaxation time-scale (Re_{l_0}) is expressed from local turbulence using the approach proposed by Fox [12] and reprised by Subramanian et al. [13]. These terms account for ensemble average variance production due to the local level of turbulence, hence they are responsible for the dispersion of physical states represented in a single fluid cell. It is important to underline that the perturbation of the local fluid state is not arbitrarily imposed, but it is derived from transport equation originating from turbulence intensity itself.

Equations 5 and 6 constitute the fundamentals of the statistical treatment of the PDF-Knock model and they extend the range of the simulated physical processes over the previously described Cell-Averaged knock model, where turbulence influence on the in-cell status was not considered.

Statistical Description of In-Cell Reaction Rate

Both cell-averaged values and their distribution around the mean (i.e. their variance) are available for enthalpy h and mixture fraction Z . As for cell-average values, these are calculated in the same way as in the model described in the previous section, i.e. from standard volume-average Navier-Stokes and transport equations, whereas local variance values are derived from the presented two additional transport equations ([Eq. 5](#) and [6](#)).

As a first step, the mixture fraction Z is examined. Given the mean value and the dispersion variance, a normal Gaussian distribution around the mean value $\bar{Z}$ in the mixture fraction space is assumed, whose spreading is represented by the local Z' variance. The probability $P(Z)$ to find the generic Z mixture quality in the cell volume is represented by [Eq. 7](#).

$$P(Z) = \frac{1}{\sqrt{Z'}\sqrt{2\pi}} \cdot \exp \left[-\frac{(Z-\bar{Z})^2}{2 \cdot Z'} \right] \quad (7)$$

If a single variable fluctuation was of interest, an analogous treatment could be carried out for enthalpy h . However, in this model both mixture fraction Z and enthalpy h are affected by turbulence through [Eq. 5](#) and [6](#) and they are expressed by the variance values h' and Z' . Their joint effect has to be accounted for in each single cell and it is evaluated using a multivariate Gaussian distribution, reported in its general form in [Eq. 8](#).

$$P(Z, h) = \frac{1}{2\pi \cdot \sqrt{Z'}\sqrt{h'}\sqrt{1-\rho^2}} \cdot \exp \left\{ -\frac{1}{2(1-\rho^2)} \cdot \left[\frac{(Z-\bar{Z})^2}{Z'} + \frac{(h-\bar{h})^2}{h'} - \frac{2\rho(Z-\bar{Z})(h-\bar{h})}{\sqrt{Z'}\sqrt{h'}} \right] \right\} \quad (8)$$

In [Eq. 8](#) ρ is the correlation coefficient between the two input variables Z and h . Since both mean values and variances are independently calculated through [Eq. 5](#) and [6](#), the two variables are considered as uncorrelated ($\rho = 0$) and [Eq. 8](#) is reduced to [Eq. 9](#).

$$P(Z, h) = \frac{1}{2\pi \cdot \sqrt{Z'}\sqrt{h'}} \cdot \exp \left\{ -\frac{1}{2} \cdot \left[\frac{(Z-\bar{Z})^2}{Z'} + \frac{(h-\bar{h})^2}{h'} \right] \right\} \quad (9)$$

As a final step, the mixture fraction space is converted into an equivalence ratio one and the unburnt temperature T_u is substituted to enthalpy through [Eq. 10](#) and [11](#).

$$T_u' = \frac{h'}{c_p} \quad (10)$$

$$\Phi' = \alpha_{st} \cdot \frac{Z'}{Y_{O_2} + Y_{N_2}} \quad (11)$$

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In Eq. 10 α_{st} is the stoichiometric air-to-fuel ratio of the fuel-air mixture, while Y_{O_2} and Y_{N_2} are the mass fractions of oxygen and nitrogen respectively. From a mathematical point of view, this treatment corresponds to a statistical reconstruction of all the possible combinations of (Φ, T_u) which can be present in the cell and whose dispersion around the mean value is given by the local turbulent time scale. The expression reported in Eq. 9 represents the probability of a given (Φ, T_u) status to exist in the cell volume. The probability is maximum for the mean values couple $(\bar{\Phi}, \bar{T}_u)$, while it is progressively reduced for far-from-average states, although it is not null for these and this anticipates the inadequacy of a single AI delay to describe the whole cell reactor. This statistical two-dimensional model for the fluid cell is graphically resumed in Figure 1.

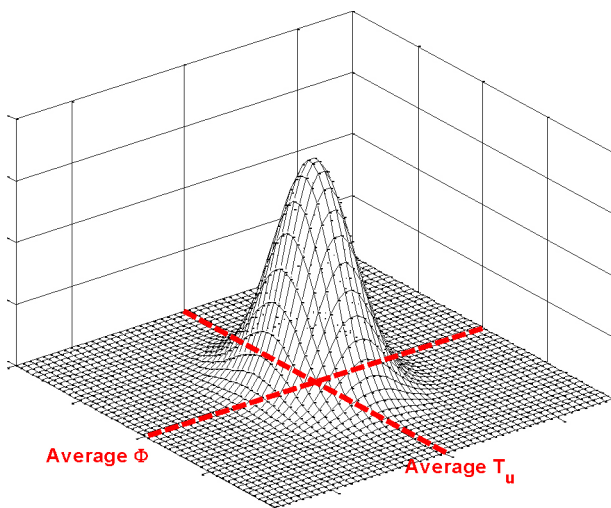


Figure 1. Multivariate Gaussian-PDF distribution of physical states for the fluid cell in the PDF-Knock model. The most probable condition $(\bar{\Phi}, \bar{T}_u)$ is represented by the intersection of the average states.

For the sake of numerical implementation, the multivariate Gaussian distribution of physical conditions (Φ, T_u) is discretized in an arbitrary number of physical conditions. In the present study a cell-wise discretization step of half of a standard deviation is adopted for both equivalence ratio and temperature, i.e. it is based on the local values of $\frac{T_u'}{2}$ and $\frac{\Phi'}{2}$. Finally, a clipping distance from the mean value must be chosen in order to bound a finite in-cell physical space: in the present analysis a clipping is adopted at twice the standard deviation of each variable, i.e. $\pm 2 \cdot \Phi'$ and $\pm 2 \cdot T_u'$. A consequence of this is that approx. the 95% of the overall probability is accounted for. This leads each of the two independent variables to be divided into 9 discrete values; therefore the distribution of the in-cell states counts 9^2 conditions. Preliminary sensitivity analyses showed that this is a balanced compromise between the resolution of the discretized distribution and the amplitude of the simulated states.

The result of the outlined procedure is a discrete clipped multivariate Gaussian distribution. The step-like discretization and the boundary truncation introduce a degree of numeric error, which alters the overall probability normalization. This effect is considered in the model and it is counterbalanced by a final re-normalization procedure designed to have the sum of the represented discrete states as equal to unity.

Knock Precursor Variance

From a general point of view, once a global reaction rate $\bar{\omega}$ is known a knock precursor increase can be calculated in the same way as the Livengood-Wu knock integral function I reported in Eq. 3.

The difference between the PDF-Knock model and the Cell-Averaged one lies in the definition of the ω term. Since a variety of physical states is statistically present in the single fluid cell, a distribution of reaction rates is also to be considered in the cell volume. The theoretical global reaction rate follows a more complex definition and it is then expressed as in Eq. 12.

$$\omega = \int_V P(\Phi, T) \cdot \omega(\Phi, T) dV = \int_V P(\Phi, T) \cdot \frac{1}{\tau(\Phi, T)} dV \quad (12)$$

The calculation of the integral can be numerically challenging, hence an assumption is made considering the dispersion of the in-cell reaction rates as the sum of a mean term and a contribution due to fluctuations. This last can be either positive or negative: it can accelerate or slow down the global reaction rate depending on the considered reaction rate, which itself depends on the local physical state. Since the focus of this study is on the earliest probability that a portion of a fluid cell experiences autoignition, just the faster-than-average part of the reaction rate spreading is of interest.

These arguments lead to the decomposition of the global reaction rate $\omega_{PDF-Knock}$ into an average value $\omega_{PDF-aver}$ and an accelerating contribution ω_{rms} (Eq. 13).

$$\omega_{PDF-Knock} = \omega_{PDF-aver} + \omega_{rms} \quad (13)$$

The former term is obtained by a PDF-weighted averaging operation of the population of reaction rates calculated on the discrete multivariate PDF space, hence the $\omega_{PDF-aver}$ name (Eq. 14).

$$\omega_{PDF-aver} = \sum_{i=1}^{\Phi_{tot}} \sum_{j=1}^{T_{tot}} P(\Phi_i, T_j) \cdot \frac{1}{\tau(\Phi_i, T_j)} d\Phi dT \quad (14)$$

The latter contribution is calculated as the difference between the $\omega_{PDF-aver}$ term and the faster-than-average reacting states considered in the discrete cell representation. It describes the root mean square of the fastest reaction rates within the fluid cell. Following an analogous $\pm 2 \cdot \tau'$ clipping for AI delays, it would correspond to an analogous representation of 95% of the statistically present states. However, a single side of the probability distribution is of interest for knock prediction, i.e. the higher than average reaction rates, therefore it expresses the reaction rate of the 2.5% fastest reacting portion (Eq. 15).

$$\omega_{+2\sigma} = \frac{1}{\tau} \Big|_{-2\sigma} \quad (15)$$

Finally the ω_{rms} term is calculated as Eq. 16 and it represents the net increase in reaction rate due to the statistical dispersion of the in-cell reaction rates.