



# A RANS knock model to predict the statistical occurrence of engine knock



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## HIGHLIGHTS

- Development of a new RANS model for SI engine knock probability.
- Turbulence-derived transport equations for variances of mixture fraction and enthalpy.
- Gasoline autoignition delay times calculated from detailed chemical kinetics.
- Knock probability validated against experiments on optically accessible GDI unit.
- PDF-based knock model accounting for the random nature of SI engine knock in RANS simulations.

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## ABSTRACT

In the recent past engine knock emerged as one of the main limiting aspects for the achievement of higher efficiency targets in modern spark-ignition (SI) engines. To attain these requirements, engine operating points must be moved as close as possible to the onset of abnormal combustions, although the turbulent nature of flow field and SI combustion leads to possibly ample fluctuations between consecutive engine cycles. This forces engine designers to distance the target condition from its theoretical optimum in order to prevent abnormal combustion, which can potentially damage engine components because of few individual heavy-knocking cycles.

A statistically based RANS knock model is presented in this study, whose aim is the prediction not only of the ensemble average knock occurrence, poorly meaningful in such a stochastic event, but also of a knock probability. The model is based on look-up tables of autoignition times from detailed chemistry, coupled with transport equations for the variance of mixture fraction and enthalpy. The transported perturbations around the ensemble average value are based on variable gradients and on a local turbulent time scale. A multi-variate 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; this results in the prediction of an earliest knock probability preceding the ensemble average knock onset, as confirmed by the experimental evidence. The proposed model estimates not only the regions where the average knock is promoted, but also where and when the first knock is more likely to be encountered.

The application of the model to a RANS simulation of a modern turbocharged direct injection (DI) SI engine with optical access is presented and the analysis of the knock statistical occurrence obtained by the proposed model adds an innovative contribution to overcome the limitation of consolidated "average knock" analyses typical of a RANS approach.

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**Abbreviations:** AI, autoignition; aSOC, After Start of Combustion; aTDC, After Top Dead Centre; BDC, Bottom Dead Centre; bTDC, Before Top Dead Centre; CA, Crank Angle; CCV, cycle-to-cycle variability; CDF, Cumulative Distribution Function; DI, direct injection; DKI, Dimensionless Knock Indicator; FSD, Flame Surface Density; GDI, Gasoline Direct Injection; IMPO, Integral Modulus of Pressure Oscillations; KLSA, Knock Limited Spark Advance; KO, knock onset; LES, Large-Eddy Simulation; MAPO, Maximum Amplitude of Pressure Oscillations; MFB, mass fraction burnt; PDF, Probability Density Function; RANS, Reynolds-Averaged Navier-Stokes; RMS, root mean square; SA, Spark Advance; SI, spark ignition; SOI, Start of Injection; TDC, Top Dead Centre; TRF, Toluene Reference Fuel.

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## 1. Introduction

In the last decades several approaches were proposed to numerically predict and simulate the average engine knock in the framework of RANS simulations. Their development was driven to meet the increasing efficiency targets requested by legislation. Thermal efficiency and specific output power are raised to unprecedented levels, in order both to reduce fuel consumption and pollutant

emissions and to simultaneously preserve the desired target performance levels.

Under high thermal loads abnormal combustion events are promoted, the most harmful of which is engine knock. Knock is the consequence of the self-ignition of a portion of unburnt mixture ahead of the main propagating flame front, and its occurrence is enhanced 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 [2] and the simultaneous random nature of the turbulent combustion typical of internal combustion engines, 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 presence 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 widely surveyed by [3–5], as well as other indicators like the DKI (Dimensionless Knock Indicator) [6] or the time-derivative of the in-cylinder pressure trace. Irrespective 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. Threshold values are part of engine manufacturer know-how and standardized limits are not defined.

All the mentioned aspects motivate why a significant research effort was paid to knock prediction in the recent years. Quasi-dimensional and three-dimensional CFD models for average knock prediction were developed and validated against experiments by several research groups. Vancollie and co-authors used a fuel-specific Arrhenius formulation for the reaction rate of methanol and ethanol fuels in [7], and the average ignition delay was used to integrate a knock precursor species. A similar modelling approach was used by Forte et al. [8] and Corti et al. in [9] for gasoline fuels.

However, the ensemble average approach to knock modelling through the use of RANS simulations suffers of the inability to reproduce the intrinsically stochastic nature of knock; this is a strong limitation for this type of models. The dramatic impact of cycle-to-cycle variability (CCV) on all the in-cylinder physical processes, such as fuel-air mixing, combustion initiation and turbulent burn rate, motivates the adoption of more refined approaches. In fact, since engine knock depends on all the preceding processes, it is itself a typically stochastic and cycle-dependent phenomenon whose accurate prediction is therefore extremely complex. A rigorous analysis of CCV can only be carried out through the use of Large-Eddy Simulation (LES), where the largest flow structures are resolved allowing the simulation of flow unsteadiness deriving from large-scale turbulence. Despite the still demanding cost of this type of analyses, several promising studies of this kind were presented in the recent years, such as the works by Robert et al. [10,11]. They showed that the simulated combustion CCV was able to replicate the degree on instability measured at the test-bench for a premixed iso-octane-air engine at several spark timings. Large-Eddy Simulation was used to predict knock occurrence in a turbocharged GDI unit by the authors in previous studies [12–14], 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. These examples showed the investigation insight made possible by LES and the possibility to explain individual misfiring cycles or cycle-specific knocking events, thus allowing a direct comparison between simulation results and engine test-bench output. However, the application of LES on production engines still suffers from the severe computational cost, preventing a full application in the design process of current units.

In this context the definition of a new approach for knock modelling emerges as a necessary bridge between the poorly representative RANS mean knock prediction and the relevant CPU effort of a multiple cycle LES study. This is based on the RANS formalism for average quantities, combined with the use of transport equations for variances of physical conditions, allowing to estimate a knock probability or a fraction of knocking cycles. The statistical RANS knock model proposed in this paper relies on transport equations for mixture fraction and enthalpy variances; detailed chemistry is used to calculate an accurate ignition delay of a gasoline surrogate model for the unburnt mixture. The variances of the variable are used as a basis of a multi-variate Gaussian model of the unburnt fluid cell, from which information on both the average reaction rate and its deviation are used to infer a presumed distribution of knocking events around the mean knock onset. An innovative definition for a probability of knocking cycles is proposed based on the same statistical basis deriving from the model equations, differently from what previously proposed by Linse et al. [15]. An initial application of the PDF-knock model was presented by the authors in [16], and the application on a knock-limited turbocharged GDI engine successfully predicted 6% of knocking cycles while the ensemble average realization was knock-safe. If a traditional RANS knock model was used, a knock-safe condition would have emerged, with no further information available on knock probability and lack of correlation with the experimental acquisitions. Conversely, the use of the presented PDF-knock model gave a quantitative information regarding the presumed fraction of knocking cycles affecting the mean simulation for a given operating condition, thus enhancing the meaning of a RANS simulation of knock with a typical test-bench acquisition dataset. This initial application motivated the development of the statistical knock model and the application on a research single-cylinder engine presented in this paper.

In the next section the details of the knock model are presented, which is based on detailed chemistry tabulation to accurately reproduce the local reaction rate. A statistically-based treatment accounting for presumed turbulence-chemistry interaction is presented and transport equations for the local perturbation of the thermal and mixing state are introduced. Finally, the derivation of the mean knock precursor and of its variance are presented. The model is applied to an optically accessible GDI engine, and the knock prediction given by the presented model is compared to the experimental outcomes in terms of frequency of knocking cycles. A criterion is also proposed to correlate the results from the Probability Density Function (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.

## 2. Presumed-PDF knock model

### 2.1. Cell-average reaction rate

The first step of the presented model is based on the calculation of a cell-wise average reaction rate. A procedure for the calculation of the autoignition (AI) delay is presented in [17,18] and it is deputed to the interpolation of a cell-specific delay time from a pre-calculated database of calculated delay times  $\bar{\tau}$ . Multi-dimensional interpolation is carried out considering the local Favre-averaged physical conditions, i.e. the input vector  $\varphi$  for the delay time interpolation considers the density-average values for each of absolute pressure, unburnt temperature, equivalence ratio and residuals mass fraction (Eq. (1)).

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

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