

# Development of a RANS-Based Knock Model to Infer the Knock Probability in a Research Spark-Ignition Engine

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## ABSTRACT

Engine knock is one of the most limiting factors for modern Spark-Ignition (SI) engines to achieve high efficiency targets. The stochastic nature of knock in SI units hinders the predictive capability of RANS knock models, which are based on ensemble averaged quantities.

To this aim, a knock model grounded in statistics was recently developed in the RANS formalism. The model is able to infer a presumed log-normal distribution of knocking cycles from a single RANS simulation by means of transport equations for variances and turbulence-derived probability density functions (PDFs) for physical quantities. As a main advantage, the model is able to estimate the earliest knock severity experienced when moving the operating condition into the knocking regime.

In this paper, improvements are introduced in the model, which is then applied to simulate the knock signature of a single-cylinder 400cm<sup>3</sup> direct-injection SI unit with optical access; the engine is operated with two spark timings, under knock-safe and knocking conditions respectively. The statistical prediction of knock resulting from the presented knock model is compared to the experimental evidence for both investigated conditions.

The agreement between the predicted and the measured knock distributions validates the proposed knock model. Finally, limitations and some unprecedented possibilities given by the model are critically discussed, with particular emphasis on the meaning of RANS knock prediction.

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## INTRODUCTION

Engine knock is the object of a huge number of studies in the recent years, as it constitutes one of the main barriers limiting the increase of efficiency for modern SI units [1,2]. Knock is caused by the self-ignition of a portion of unburnt mixture before the main flame front initiated by the spark-plug regularly consumes it in deflagration mode. The sudden and simultaneous heat release of the remaining end-gas mixture may trigger a detonating pressure wave within the combustion chamber and severely damage engine components, thus preventing engine reliability. Knock-safe conditions are typically pursued through a combination of boosting limitation, charge enrichment and SA reduction. All these remedies relevantly affect engine-out performance and efficiency.

From a modelling standpoint, the stochastic nature of engine knock, related to combustion instability and cycle-to-cycle variability (CCV) of turbulent flows, would suggest Large-Eddy Simulation (LES) as

the most appropriate approach for CFD simulations. Despite this is conceptually true and several publications show the applicability of LES to both research and production units [3, 4, 5, 6, 7, 8, 9], LES still remains a very demanding approach which can hardly be integrated in the industrial design process for the development of new SI units.

To limit computational costs and times, RANS models are usually chosen to represent the average engine behavior. Several successful knock models are available in literature to predict average knock onset in SI engines [10,11], though they all suffer from the intrinsic inability to account for far-from-average realizations. This limitation can be overcome by the use of variance equations for fundamental physical variables in RANS, such as in the models proposed by Linse et al. [12] and by the authors [13]. The information given by this kind of models is of statistical nature and it is grounded in turbulence-generated variance of physical fields, which in turn affects the end-gas reaction rate towards auto-ignition. Conversely from LES

these models naturally neglect a series of CCV-promoting factors, e.g. those pertaining to variability in spark-ignited flame kernel onset and turbulent flame propagation variability. However, such statistics-based RANS models are able to artificially reconstruct a presumed probability of knocking cycles, which can be a very useful indication to the engine designer. Finally, the presumed probability of knocking cycles deriving from this family of models can be correlated to the response of knock controllers, allowing a physically more robust knock analysis than that using consolidated models based on average quantities only.

In [13] the authors proposed an early version of such PDF-based knock model, considering the in-cell variation of temperature and mixture fraction. This was the basis for a Gaussian representation of knock onset probability, and ultimately for the reconstruction of a presumed fraction of knocking cycles. In the present paper, the PDF-knock model is further developed and several improvements are introduced. A first one involves the statistical link for the in-cell conditions between temperature and mixture quality variations: a dynamically calculated correlation coefficient between mean fields of mixture fraction and temperature is now introduced.

A second one is the function used for the knock probability reconstruction. In particular, log-normal distributions are adopted as the most representative univariate distribution function for knock onset. Similar distributions were used in several experimental studies analyzing knock onset results, such as those by Peyton Jones and co-workers [14, 15, 16, 17, 18, 19]. They demonstrated that for low-to-moderate knock intensities, engine knock is essentially a cyclically independent phenomenon and no cycle-to-cycle correlation is present for a wide variety of engine speeds and loads. Independently of the metrics used to identify knock intensity, log-normal distribution is found to be a good candidate to represent the rate of probability of knocking events of a given severity. In fact, a vast majority of the population of cycles usually lies in a restricted region around the mean knock intensities, though a “longer tail” of sporadic but damaging knocking individuals is observed. This becomes more and more relevant as the engine operating condition is moved towards knock-affected conditions and the distribution of knock intensities becomes more and more spread. The fraction of knocking cycles is found to increase rapidly with SA increase, thus preventing the engine operation at edge-of-knock conditions. Such behavior was observed for several engine conditions, either knock-safe and knocking ones; in order to describe this evidence some kind of non-symmetrical distribution function is needed. In this framework, log-normal functions were found to be a useful tool. Finally, the related Cumulative Density Function (CDF) is used to describe the overall probability to exceed a predefined knocking threshold, which can be easily related to the fraction of knocking cycles.

In the next Section, the PDF-Knock model details are reported, with particular care to the modelling improvements introduced from the model in [13]. Then the model will be applied at first to a simple test case, to highlight all the main parameters behavior, and then to a research engine tested at different SA. Finally, considerations on the knock probability presumed distribution indicated by the PDF-Knock model will be critically discussed.

## PDF-KNOCK MODEL

The presented PDF-Knock model is a development of the approach proposed originally in [13]. It is recalled here in its fundamentals, together with the description of the model improvements.

### Motivations for the PDF-Knock Model

The standard approach to knock modelling considers the Livengood-Wu knock precursor  $I$  [20] to track the progress towards autoignition (Eq. 1); such approach is based on a unique cell-averaged ignition delay time  $\bar{\tau}$  and its inverse (i.e. the cell-averaged reaction rate  $\bar{\omega}$ ). The AI delay time is calculated using the look-up table approach proposed by the authors [10] which considers  $\bar{\tau}$  as a function of mean cell quantities, i.e.  $\bar{\tau} = \bar{\tau}(\bar{p}, \bar{T}_u, \bar{\Phi}, \bar{Y}_{EGR})$ . To this aim, an indexed look-up table containing chemistry calculated ignition delay times from a detailed chemical mechanism is generated off-line and it is recalled during the CFD run.

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

However, this framework fails if in-cell variability of physical states is considered, since a global cell-averaged reaction rate  $\bar{\omega}$  is not uniquely defined. To overcome this limitation, the use of multiple knock precursors will be advocated.

### PDF-Knock Model Equations

As stated before, the model is based on two additional transport equations for the variance of both mixture fraction  $Z$  and temperature  $T$ . Since both quantities affect the local AI delay time, it is inferred that their statistical variance (if present) should have an impact also on the in-cell description of the AI reaction rate.

The two additional transport equations for the variance of  $Z$  and  $T$ ,  $Z'$  and  $T_u'$  respectively, are reported below (Eq. 2 and 3).

$$\frac{\partial \rho Z'}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho v_j Z' - \left( \rho D_{Z'} + \frac{\mu_t}{\sigma_t} \right) \frac{\partial Z'}{\partial x_j} \right] = 2 \frac{\mu_t}{\sigma_t} \left( \frac{\partial Z}{\partial x_j} \right)^2 - c_t \rho \frac{\varepsilon}{k} Z' \quad (2)$$

$$\frac{\partial \rho T_u'}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho v_j T_u' - \left( \rho D_{T_u'} + \frac{\mu_t}{\sigma_t} \right) \frac{\partial T_u'}{\partial x_j} \right] = 2 \frac{\mu_t}{\sigma_t} \left( \frac{\partial T_u}{\partial x_j} \right)^2 - c_t \rho \frac{\varepsilon}{k} T_u' \quad (3)$$

It is to be noted that the Favre-averaged energy equation solved by the CFD code is in the form of sensible enthalpy, from which the conversion to temperature is possible thanks to the local mixture specific heat. This is calculated based on local species composition. As for energy variance, the temperature formulation (Eq. 3) is adopted. In Eq. 2 and 3 a fixed turbulent Schmidt number  $\sigma_t$  equal to 0.9 is used. These equations differ from their counterparts for the mean quantities

$\bar{Z}$  and  $\bar{T}_u$  in the right-hand side (RHS) terms, formally source terms for the variance equations.

The first RHS contribution is a positive source (i.e. variance generation) and it accounts for variance produced by the spatial gradient of the variable. The second RHS term describes variance dissipation, which is a function of a turbulent relaxation time-scale time scale  $\tau_t$ , reported in Eq. 4:

$$\tau_t = \frac{1}{c_t(Re_t)} \cdot \frac{k}{\varepsilon} \quad (4)$$

The characteristic turbulent time-scale of the  $k - \varepsilon$  turbulence model (i.e.  $k/\varepsilon$ ) is multiplied by a model constant  $c_t(Re_t)^{-1}$ . This is calculated as a monotonic increasing function of the local turbulent Reynolds number  $Re_t$ , as suggested by Fox [21] and by Subramanian et al. [22]. The  $c_t(Re_t)$  value is cell-wise calculated from the curve reported in Figure 1.

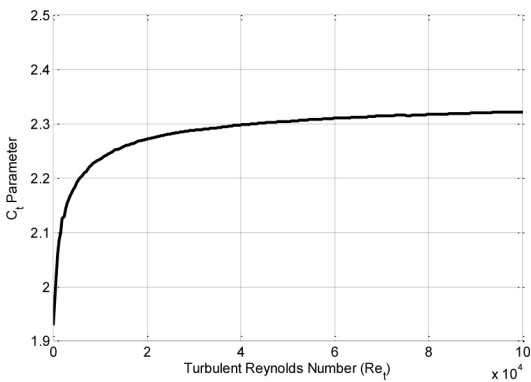


Figure 1. Variance dissipation parameter  $c_t(Re_t)$ .

Low turbulent level (i.e. low  $Re_t$ ) implies a small value of  $c_t(Re_t)$ , this in turn resulting in a long turbulent relaxation time-scale  $\tau_t$  from Eq. 4. As a consequence, the variance destruction operated by turbulent mixing in Eq. 2 and 3 is slow and the probability to find far from average in-cell states is high. The opposite situation characterizes highly turbulent conditions, where intense thermomechanical turbulent mixing leads to high  $c_t(Re_t)$  values, low relaxation time-scale  $\tau_t$  and a rapid and effective variance destruction; the system moves therefore towards a perfectly stirred status. Finally, the variance dissipation source term is proportional to the variance intensity itself.

### Statistical Model for the In-Cell Conditions

In a perfectly homogeneous field, the first RHS term would be null, since no variable gradients are present and variance could not be generated. In the same situation, there would be no possible variance dissipation as well, since this would be proportional to the variance itself. To satisfy both conditions, variance must be identically null in every point. This describes the variance equations behavior for a singular case such as a perfectly homogeneous field. For inhomogeneous fields, both the first and the second moments (i.e. the mean and the variance) for mixture fraction  $Z$  and unburnt temperature  $T_u$  are generally not null. As presented in [13], the joint variation of both variables may be represented as a simplified Gaussian bi-variate distribution model, expressed by Eq. 5:

$$P(Z, T) = \frac{1}{2\pi\sigma_Z\sigma_{T_u}} \cdot \exp\left\{-\frac{1}{2} \cdot \left[\frac{(Z-\bar{Z})^2}{\sigma_Z^2} + \frac{(T_u-\bar{T}_u)^2}{\sigma_{T_u}^2}\right]\right\} \quad (5)$$

However, Eq. 4 is valid under the assumption of uncorrelated  $Z$  and  $T_u$  variables, which is an unlikely scenario for modern GDI units, where intense fuel stratification is observed. Charge stratification usually persists until the end of the compression stroke, and it causes temperature inhomogeneity due to the dependency of the specific heat on mixture quality.

In the present paper the model is improved by considering a more refined scenario where this correlation exists and influences the shape of the bi-variate statistical model for the in-cell physical states.

To this aim, the model is evolved by considering the general formulation for bi-variate Gaussian distribution, reported in Eq. 6 and by introducing a correlation coefficient  $\rho_{ZT}$ :

$$P(Z, T) = \frac{1}{2\pi\sigma_Z\sigma_{T_u}\sqrt{1-\rho_{ZT}^2}} \cdot \exp\left\{-\frac{1}{2(1-\rho_{ZT}^2)} \cdot \left[\frac{(Z-\bar{Z})^2}{\sigma_Z^2} + \frac{(T_u-\bar{T}_u)^2}{\sigma_{T_u}^2} - \frac{2\rho_{ZT}(Z-\bar{Z})(T_u-\bar{T}_u)}{\sigma_Z\sigma_{T_u}}\right]\right\} \quad (6)$$

This formulation accounts for correlated  $Z$  and  $T_u$  variables. The correlation coefficient  $\rho_{ZT}$  is calculated in the model at each iteration through the analysis of the in-cylinder instantaneous

$\tilde{Z}$  and  $\tilde{T}_u$  fields and it is modelled using a Pearson-like formulation as in Eq. 7:

$$\rho_{ZT} = \frac{\sigma_{ZT}}{\sigma_Z\sigma_{T_u}} = \frac{\sum_i[(Z_i-\bar{Z})(T_{u,i}-\bar{T}_u)]}{\sqrt{\sum_i(Z_i-\bar{Z})^2} \cdot \sqrt{\sum_i(T_{u,i}-\bar{T}_u)^2}} \quad (7)$$

In Eq. 7, the  $\sigma_Z$  and  $\sigma_{T_u}$  terms are the standard deviation of the mean in-cylinder  $\tilde{Z}$  and  $\tilde{T}_u$  fields. Therefore, the  $\rho_{ZT}$  coefficient is dynamically calculated at each iteration based on the instantaneous modeled mean  $\tilde{Z}$  and  $\tilde{T}_u$  fields and it is found to be always negative: high  $\tilde{Z}$  cell-values (i.e. rich-in-fuel regions) are more likely associated to low  $\tilde{T}_u$ . This is an expected consequence of the relationship between  $\tilde{Z}$  and  $\tilde{T}_u$  deriving from the mixture isobaric specific heat. The instantaneous local  $\rho_{ZT}$  correlation coefficient modifies the bi-variate Gaussian model for the in-cell conditions as illustrated in Figure 2 for several  $\rho_{ZT}$  parameter values. In Figure 2 the equivalence ratio is used instead of  $\tilde{Z}$  to represent fuel concentration. Hotter states are associated with leaner mixtures (bottom-right side in Figure 2) and the same is for cooler and richer conditions (upper-left side in Figure 2), while hot and rich (upper-right) or cool and lean (lower-left) combinations are less probable.

Finally, it is noted that bi-variate Gaussian distribution is one of the possible models for the cell reactor model and it could be substituted by bi-variate beta-distribution. The authors choice of bi-variate Gaussian distribution is motivated by its relative simplicity and its robust representation of in-cell distribution of states.

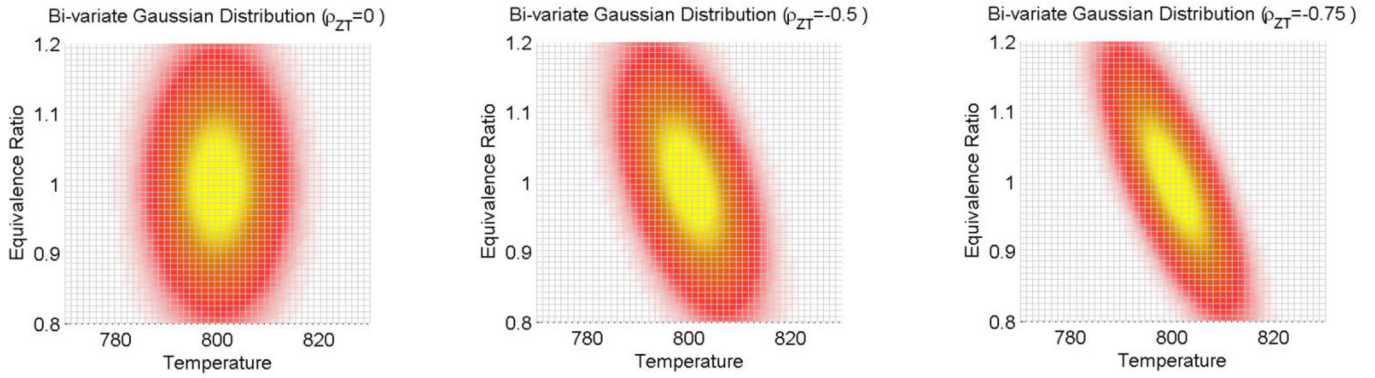


Figure 2. Bi-variate Gaussian distribution for the in-cell statistical states as a function of the  $\rho_{ZT}$  correlation coefficient:  $\rho_{ZT} = 0$  (left, uncorrelated equivalence ratio and  $T_u$ ),  $\rho_{ZT} = -0.5$  and  $\rho_{ZT} = -0.75$  (middle and right, negatively correlated equivalence ratio and  $T_u$ ).

### Statistical Model for the In-Cell Reaction Rate

Given the outlined model to represent the statistical distribution of in-cell conditions, a similar treatment based on first and second moments is pursued for the description of the reaction rate distribution.

In fact, once in-cell variability of physical states is introduced, a unique cell-averaged ignition delay time  $\tilde{\tau}$  (or the cell-averaged reaction rate  $\tilde{\omega}$ ) is not sufficiently representative of the cell reactivity states. To overcome this limitation, multiple knock precursors are adopted.

The mean ignition delay  $\tau_{PDF-aver}$  is calculated as the PDF-weighted average of the ignition delay times of all the in-cell represented conditions (Eq. 8), from which a cell-average reaction rate  $\omega_{PDF-aver}$  is derived (Eq. 9).

$$\tau_{PDF-aver} = \sum_{i=1}^{Z_{tot}} \sum_{j=1}^{T_{u,tot}} P(Z_i, T_{u,j}) \cdot \tau(Z_i, T_{u,j}) dZ dT_u \quad (8)$$

$$\omega_{PDF-aver} = \tau_{PDF-aver}^{-1} \quad (9)$$

The weighting operator is the bi-variate Gaussian model reported in Eq. 6, accounting for  $\tilde{Z}$  and  $\tilde{T}_u$  mutual correlation through  $\rho_{ZT}$  (Eq. 7). The role of the  $\omega_{PDF-aver}$  term is similar to the standard reaction rate for the knock precursor in RANS knock models, i.e. conceptually accounting for the mean precursor growth towards knock as if the entire cell was at its Favre-average status. It is however to be noted that even if  $\omega_{PDF-aver}$  is a mean term, it is calculated by weighting on all the represented states in the cell, hence non-linear  $\tau$  variation are considered.

As a second step, a variance-like variable must be introduced to represent the reaction rate distribution around the PDF-weighted average value. However, differently from the previous model implementation in [13], attention is paid to the reaction rate distribution emerging from this treatment. In fact, different variance amplitudes are encountered if distribution spread is calculated on the faster or slower-than-average states: in other words, the in-cell distribution of reaction rates does not rigorously follow a normal distribution. This is due to the rapid AI delay decrease when entering in the medium-to-high temperature chemistry, while much slower reacting states are still present for slightly lower  $T_u$ . As a model improvement, this behavior is accounted for by two conditioned

variances calculated for each cell: one for the faster-than-average states and one for the slower-than-average,  $\sigma_{\tau,-\sigma}$  and  $\sigma_{\tau,+\sigma}$  respectively (Eq. 10 and 11).

$$\sigma_{\tau,-\sigma} = \sqrt{\frac{1}{N} (\tau_i - \tau_{PDF-aver})^2} \Big|_{\tau_i < \tau_{PDF-aver}} \quad (10)$$

$$\sigma_{\tau,+\sigma} = \sqrt{\frac{1}{N} (\tau_i - \tau_{PDF-aver})^2} \Big|_{\tau_i > \tau_{PDF-aver}} \quad (11)$$

Based on these quantities, it is possible to calculate the net difference in reaction rate from the mean value  $\omega_{PDF-aver}$ . Two variables are used for this,  $\tau_{-\sigma}$  and  $\tau_{+\sigma}$  respectively, representing the ignition delay difference from the mean value  $\tau_{PDF-aver}$  and calculated as in Eq. 12 and 13.

$$\tau_{-\sigma} = \tau_{PDF-aver} - \sigma_{\tau,-\sigma} \quad (12)$$

$$\tau_{+\sigma} = \tau_{PDF-aver} + \sigma_{\tau,+\sigma} \quad (13)$$

Finally, two reactions rates are calculated,  $\omega_{-\sigma}$  and  $\omega_{+\sigma}$ , representing the reaction rate acceleration and slow-down with respect to the mean  $\omega_{PDF-aver}$  (Eq. 14 and 15).

$$\omega_{-\sigma} = \frac{1}{\tau_{-\sigma}} - \frac{1}{\tau_{PDF-aver}} = \frac{\tau_{PDF-aver} - \tau_{-\sigma}}{\tau_{PDF-aver} \cdot \tau_{-\sigma}} \quad (14)$$

$$\omega_{+\sigma} = \frac{1}{\tau_{+\sigma}} - \frac{1}{\tau_{PDF-aver}} = \frac{\tau_{PDF-aver} - \tau_{+\sigma}}{\tau_{PDF-aver} \cdot \tau_{+\sigma}} \quad (15)$$

Since  $\omega_{-\sigma}$  is a positive contribution, being  $\tau_{PDF-aver} > \tau_{-\sigma}$ , it represents a reaction rate deviation towards an earlier autoignition event. By the same rationale,  $\omega_{+\sigma}$  is a negative contribution, since  $\tau_{PDF-aver} < \tau_{+\sigma}$ , and it accounts for a statistically existing reduced reaction rate.

As last step, three independent knock precursors are transported, all based on a Livengood-Wu model. The first knock precursor  $I_{PDF-aver}$  represents a Livengood-Wu model for the cell-average reaction rate, whose transport equation is Eq. 16:

$$\frac{\partial \bar{p} I_{PDF-aver}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{v} I_{PDF-aver}) = \nabla \cdot (\bar{\rho} (D + D_T) \nabla I_{PDF-aver}) + \bar{\rho} \omega_{PDF-aver} \quad (16)$$

The other two reaction rates,  $I_{-\sigma}$  and  $I_{+\sigma}$ , follow a similar modeling approach, the only conceptual difference with  $I_{PDF-aver}$  being their meaning: they represent the net difference of the knock precursor from the average one. Their transport equations are Eq. 17 and 18, and their source terms are  $\omega_{-\sigma}$  and  $\omega_{+\sigma}$  (Eq. 14 and 15) respectively. These are calculated based on turbulence-generated deviation of physical states (and consequently of AI delay times), hence they are dependent upon flow features only and not derived by user-imposed alteration of fields.

$$\frac{\partial \bar{p} I_{-\sigma}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{v} I_{-\sigma}) = \nabla \cdot (\bar{\rho} (D + D_T) \nabla I_{-\sigma}) + \bar{\rho} \omega_{-\sigma} \quad (17)$$

$$\frac{\partial \bar{p} I_{+\sigma}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{v} I_{+\sigma}) = \nabla \cdot (\bar{\rho} (D + D_T) \nabla I_{+\sigma}) + \bar{\rho} \omega_{+\sigma} \quad (18)$$

In the next Section it will be shown how the introduced knock precursors are used to reconstruct a presumed probability of knocking cycles.

### Probability of Knocking Cycles

As stated in the Introduction, the analysis of knocking conditions is severely limited by the underlying assumptions of the RANS formalism, namely the phase-averaging of Navier-Stokes equations preventing a detailed simulation of stochastic events which can only be accounted for by statistical models.

In [13] the authors used the mean knock precursor and its variance to define a PDF distribution of knocking cycles. From this, a CDF was calculated to presume a probability of knocking cycles.

In this study the PDF-Knock model is evolved from [13] by considering log-normal distribution as a more consistent representation than normal Gaussian shape, as outlined in the Introduction section [14,15]. Log-normal distribution of probability  $P(x)$  of a strictly positive  $x$  variable is defined as in Eq. 19:

$$P(x) = \frac{1}{x \cdot \sigma \sqrt{2\pi}} \cdot e^{-\frac{(\ln x - \mu)^2}{2\sigma^2}} \quad (19)$$

In Eq. 19  $\mu$  and  $\sigma$  are the mean and standard deviation of the  $\ln(x)$  distribution, and they represent a location and a scale parameter. The mean value and the standard deviation of  $x$ ,  $M$  and  $v$  respectively, are defined as Eq. 20 and 21.

$$M = e^{\mu + \frac{\sigma^2}{2}} \quad (20)$$

$$v = (e^{\sigma^2} - 1) \cdot e^{2\mu + \sigma^2} \quad (21)$$

Therefore, a method is proposed to correlate CFD results to distribution parameters. This is based on two knock phasing indicators,  $MFU_{\overline{KO}}$  and  $MFU_{KO'}$ : they both express the residual unburnt fuel fraction at knock onset. As for  $MFU_{\overline{KO}}$ , it is related to the average knock phasing: it represents the unburnt fraction at mean knock onset as indicated by the  $I_{PDF-aver}$  precursor reaching unity value. Similarly,  $MFU_{KO'}$  regards the same quantity at knock onset as indicated by the  $I_{-\sigma}$  precursor. Given the three-dimensional nature of the  $I_{PDF-aver}$  and  $I_{-\sigma}$  fields, knock onset is considered as the instant at which  $I_{PDF-aver}$  or  $I_{-\sigma}$  exceed 1 mm<sup>3</sup> of volume with value higher than unity.

Coherently with the RANS meaning for mean and variance, the mean value  $M$  is taken as the residual burnt fraction at knock onset, i.e.  $MFU_{\overline{KO}} = 1 - MFB_{\overline{KO}}$ , while the standard deviation  $v$  is given by the difference in burnt fraction between the earliest knock onset  $KO'$  and the mean one  $\overline{KO}$ . Therefore the linear system (Eq. 22 and 23) is defined as:

$$M = MFU_{\overline{KO}} = e^{\mu + \frac{\sigma^2}{2}} \quad (22)$$

$$v = MFU_{KO'} - MFU_{\overline{KO}} = (e^{\sigma^2} - 1) \cdot e^{2\mu + \sigma^2} \quad (23)$$

The two equation system in two unknowns ( $\mu$  and  $\sigma$ ) is solved and expressions for the log-normal parameters are obtained as Eq. 24 and 25, describing a presumed log-normal distribution of knocking events based on the PDF-Knock model outcomes  $MFU_{KO'}$  and  $MFU_{\overline{KO}}$ .

$$\sigma = \sqrt{\ln[1 + MFU_{KO'} \cdot e^{-2 \cdot \ln(MFU_{\overline{KO}})}]} \quad (24)$$

$$\mu = \ln(MFU_{\overline{KO}}) - \frac{\sigma^2}{2} \quad (25)$$

Finally, the fraction of knocking cycles is calculated as the Cumulative Density Function (CDF) of Eq. 19, expressed by Eq. 26:

$$CDF(x) = \frac{1}{2} \cdot \left[ 1 + \operatorname{erf} \left( \frac{\ln x - \mu}{\sigma \sqrt{2}} \right) \right] \quad (26)$$

This represents the cumulative probability to have knocking events for a given  $MFU_{KO'}$ . Since many knock intensity indicators are used and their specific threshold are based on manufacturers' experience, a more general knock severity indicator is assumed here as the  $MFU_{KO'}$ . Knock intensity is commonly related to the residual burnt fraction at knock [23], and a distribution of this last can be used to infer an overall probability to record knocking events up to a given threshold. Finally, the complement to one is the cumulative probability to exceed such value, i.e. the statistical fraction of knocking cycles.

Given the model aim to comprehensively predict a presumed probability of knocking events, heat released by autoignition is numerically de-activated: it would be conceptually wrong to generate heat by one singular event (e.g. the earliest knock probability), thus altering the remaining realizations (e.g. the average knock onset) by thermodynamic effects.

## PDF-KNOCK MODEL TEST CASE

A simple test case is illustrated in order to highlight the PDF-Knock model behavior for engine-typical conditions. A finite size rectangular plane is initialized with constant absolute pressure and temperature, 70 bar and 900 K respectively. As for species concentrations, a stoichiometric Gasoline field is imposed with no EGR presence.

The plane is initialized with increasing temperature variance  $T_u'$  on the x-direction, while increasing  $Z'$  is imposed on the y-direction. This variance initialization serves as a substitute of the transport equations for variances (Eq. 2 and 3 for  $T_u'$  and  $Z'$ ) and it is here adopted for test purposes only. The variance initial fields are illustrated in Figure 3.

As a result, the lower-left corner corresponds to a perfect-stirred reactor (PSR) condition (Point A) with no in-cell variance, while the upper-right corner to a highly variant condition (Point B). These are typical situations for high-turbulent (Point A) and low-turbulent states (Point B). The bi-variate PDF representing Point A and B states are represented in Figure 4. Given the identical mean  $Z$  and  $T_u$  fields used for this test case, the  $\rho_{ZT}$  correlation coefficient is not defined and the bi-variate model is built considering the simplified formulation for  $\rho_{ZT} = 0$  (Eq. 5).

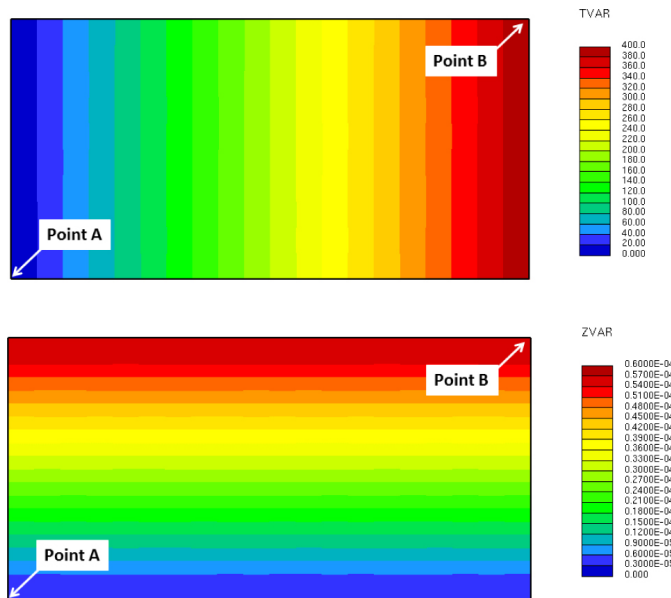


Figure 3. Variance initial fields for the test case: unburnt temperature variance  $T_u'$  (top) and mixture fraction  $Z'$  variance (bottom).

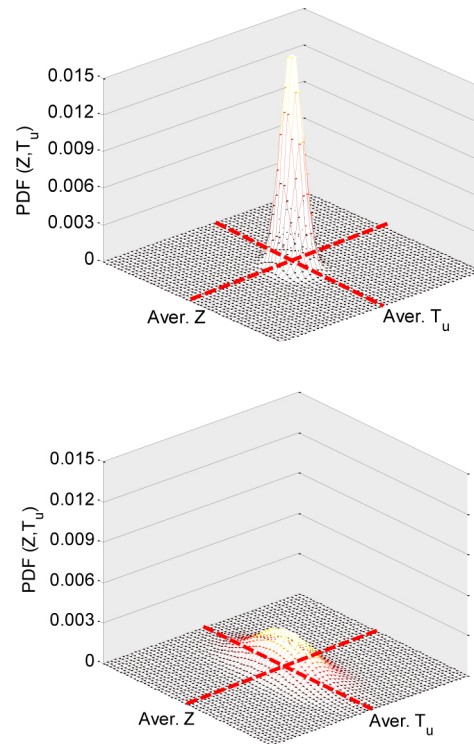


Figure 4. Probability Density Function of mixture fraction and unburnt temperature for Point A (Perfectly Stirred Reactor, top) and Point B (highly variant status, bottom).

Given the identical average pressure, temperature and mean mixture quality, the mean reaction rate for the analysed conditions would indicate a time to autoignition equal to 0.86 ms for a RON95 gasoline. However, the PDF treatment on temperature and mixture fraction considers the statistical deviation of such physical conditions from the mean values, hence a reaction rate distribution arises moving from Point A (equal reaction rate over the entire cell volume) to Point B.

In Figure 5 the PDF-weighted average delay time  $\tau_{PDF-aver}$  and the separate standard deviations  $\sigma_{\tau-\sigma}$  and  $\sigma_{\tau+\sigma}$  are reported at 0.86 ms. It is visible that while  $\tau_{PDF-aver}$  is roughly uniform, due to the identical mean conditions, AI delay variability is null at Point A and maximum at Point B.

The mean source term  $\omega_{PDF-aver}$  field (Eq. 9) is represented in Figure 6 (left) and it is little affected by the increasing field variance moving from the lower-left to the upper-right corner. However, the in-cell presence of far-from-average states induces a reaction rate variance, represented in Figure 6 in terms of  $\omega_{-\sigma}$  and  $\omega_{+\sigma}$  respectively; both fields show null values at Point A (homogeneous PSR condition) and peak values at Point B (highly variant state). As previously underlined,  $\omega_{-\sigma}$  has a positive sign while  $\omega_{+\sigma}$  is negative.

The final result of the PDF treatment is that a statistically earlier knock onset is introduced together with the average knock prediction, and this depends on the variance amplitude. The knock precursor fields for the average knock precursor  $I_{PDF-aver}$  is reported in Figure 7 at 0.9 ms, as well as its higher and lower values given by the  $I_{-\sigma}$  and  $I_{+\sigma}$  effect. As visible, the maximum deviation from the average knock