

Super-Knock Prediction Using a Refined Theory of Turbulence

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ABSTRACT

The occurrence of severe events of ‘super-knock’ originating from random pre-ignition kernels which sometimes is observed in turbo-charged spark-ignition engines was recently attributed by Kalghatgi and Bradley [4] to developing detonations which originate from a resonance between acoustic waves emitted by an auto-igniting ‘hot spot’ and a reaction wave which propagates along negative temperature gradients in the fuel-air mixture. Their occurrence depends on the steepness of the local instantaneous temperature gradient and on the length of the region of negative gradient. The theory requires that the temperature gradient extends smoothly over a sufficient length in the turbulent flow field. Then localized detonations may develop which are able to autoignite the entire charge within less than a millisecond and thus cause pre-ignition and ‘super-knock’.

In this paper we ascribe the stochastic occurrence of preignition and the resulting ‘super-knock’ events to the stochastic nature of turbulence. The detonation diagram proposed by Kalghatgi and Bradley [4] is combined with the results of a refined theory of small scale turbulence developed recently by the group of the first author. That theory - differently from traditional theories of turbulence - can predict the joint probability density of smooth temperature gradients and the length over which they extend. The joint probability density is obtained from Direct Numerical Simulations. It becomes universal when it is normalized by traditional turbulence quantities as they are used in CFD simulations. The detonation limits in the diagram of [4] will serve as integration limits when the joint probability density is integrated to obtain a detonation probability. Numerical CFD simulations of motored cycles for turbo-charged engines show that the highest detonation probabilities occur in localized regions in the bulk of the combustion chamber where the flow is rather uniform and where therefore the integral time scale is large. In these regions there is a high probability of a large local length over which a reaction wave can travel.

The simulations predict a larger cycle probability for higher boost pressures, higher intake air and wall temperatures, lower engine speeds and lower octane numbers, if all the other boundary conditions remain the same. A higher spark plug temperature did not lead to an increase of pre-ignition probabilities.

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INTRODUCTION

Modern highly downsized spark ignition engines may produce a very high IMEP and thereby reduce the fuel consumption considerably. A drawback of this technology is the occurrence of sporadic pre-ignition kernels leading to violent ‘superknock’ events which can damage the moving parts of the engine. This abnormal combustion is all the more dangerous as it cannot be avoided by simply retarding the spark timing or reducing the fuel-to-air ratio as it is generally done to avoid the classical knock phenomenon. Dahnz and Spicher [1] have discussed the irregular combustion

phenomena occurring in super-charged spark ignition engines, namely classical knock, extreme knock, surface ignition and pre-ignition, and have evaluated them in terms of their severity. While knock sensors employed in modern engines can reduce the occurrence of classical knock by retarding the spark advance, extreme knock occurring at high engine speeds and exhibiting significantly higher amplitudes, can not be avoided by standard knock control. Surface ignition is the result of repeated knock events which heat up the engine walls and consequently the combustion chamber. In principle it can be avoided by appropriate cooling of the walls and by the right choice and position of the spark plug.

The last phenomenon, pre-ignition, which takes place prematurely before the spark and occurs particularly in highly supercharged downsized engines, is described in [1] as relatively new and the least understood. It resembles extreme knock and surface ignition in its severity for the engine, but is not self-amplifying as surface ignition. It occurs stochastically, just like extreme knock.

Also, in order to relate the pre-ignition frequency to parameters which can be varied in real engines, Dahnz and Spicher [1] reported variations of the inlet air temperature and the cooling water temperature and of the fuel used. While no specific trend could be determined by changing the air temperature from 13 °C to 30 °C, the rise of the cooling water temperature from 75 °C to 95 °C would reduce the preignition frequency from approximately 20 to 10 events in 10,000 cycles. Changing the Research octane number (RON) from 95 to 100 would reduce it by the same amount. A hypothesis is formulated which explains the decrease of the pre-ignition frequency with increasing cooling water temperature and increasing RON. It ascribes the occurrence of pre-ignition to the presence of highly ignitable droplets containing lubricant oil which are stripped randomly from the cylinder walls. Also fuel droplets entrained from the top land of the piston would be able to initiate random ignition kernels that eventually lead to strong pressure increases.

In a comprehensive experimental and theoretical approach Zahdeh et al. [2] have identified several parameters which may have a direct effect on the onset of pre-ignition including liner wetting, injection targeting, mixture stratification, mixture motion and oil formulation. Among these injection targeting is found to be most crucial. They suggest that oil mixing with the fuel would lower the self-ignition temperature and would hence cause premature combustion. A 3-D model of piston ring dynamics was developed to understand the stochastic nature of oil intrusion into the combustion chamber. Nevertheless the authors note that the mechanism of oil and fuel accumulation to produce self-ignition is not fully understood. They also note that a sufficiently high end of compression temperature has to be met for pre-ignition to take place.

Zaccardi et al. [3] investigate the effects of in-cylinder charge motions on pre-ignition probabilities for direct injection (DI) and port fuel injection (PFI) and for medium and high tumble cases and a mix of swirl and tumble. Pre-ignition probabilities are found to decrease with increasing engine speeds between 1000 and 2000 rpm for both injection modes and both tumble configurations. For the high tumble case the DI mode reduces the pre-ignition probability for the lower IMEP cases. The probabilities were further reduced to less than 1% when high swirl is added to the tumble.

Kalghatgi and Bradley [4] give an historical account of the damaging effects of pre-ignition and the resulting 'super-knock' due to turbo-charging and then move to present hypotheses and the ongoing discussions thereof. They summarize the recent literature by noting that pre-ignitions are characterized by:

- a. higher pressures and temperatures that spasmodically give rise to gas-phase pre-ignitions;
- b. auto-ignitions at even higher pressures and temperatures that might cause very severe, damaging knock;
- c. injector sprays striking surrounding surfaces and stripping lubricating oil from them;
- d. lubricating oil and fuel mixing with the main hot charge and auto-igniting due to lower ignition temperature;
- e. residual gas or particles creating gas phase 'hot spots';
- f. different pre-ignition rankings of different fuels.

With respect to auto-ignitive pre-ignition they argue that in modern engines pre-ignition is unlikely to be initiated at internal surfaces. They also dismiss suggestions by Zadeh et al. [3] and Dahnz and Spicher [1] that oil or fuel droplets would be responsible for pre-ignition. They maintain that from such igniting droplets premixed turbulent flames would propagate just as if they had been initiated by the spark. In order to cause super-knock an auto-igniting gas phase 'hot spot' would need to be reinforced by another mechanism, namely the acoustic coupling between the reaction wave that it initiates and the sound wave that it emits. For this to happen the reaction wave must be traveling along a negative temperature gradient over a sufficiently long distance. Under certain conditions this could lead to a localized developing detonation and hence to 'super-knock'.

THEORETICAL BACKGROUND

In this paper we will follow Kalghatgi and Bradley [4] who argue that auto-ignition is a necessary but not sufficient condition for pre-ignition. Bradley et al. [5] and Gu et al. [6] had developed a comprehensive theory of wave amplification and Bradley and Kalghatgi [7] had considered the effect of different fuels on engine knock. The analysis is based on a prediction by Zeldovich [8] who distinguishes between several modes of propagation of reaction waves in mixtures with temperature gradients. A developing detonation is postulated to occur as an acoustic resonance phenomenon between the reaction wave velocity and the sound speed a . The analysis requires that the temperature derivative of the ignition delay time τ couples locally with a negative spatial temperature gradient $\partial T/\partial x$ in direction of the front propagation in such a way that a large (positive) front velocity u results

$$u = 1/(\mathrm{d}\tau/\mathrm{d}T * \partial T/\partial x) . \quad (1)$$

If this velocity is of the order of magnitude of the sound speed a , there is the possibility that a detonation wave develops.

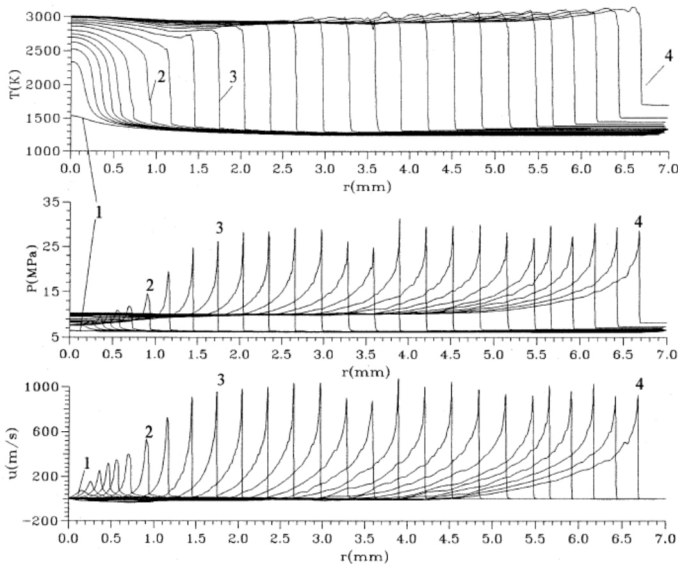


Figure 1. The profiles of temperature, pressure and velocity calculated from a one-dimensional simulation performed in [6] for an H_2 -CO-air mixture. The ratio of the sound speed to the front propagation velocity was 3. In this case a detonation develops.

In [6] several different propagation scenarios were analyzed for a H_2 -CO-air mixture, one of which led to a developing detonation as shown in figure 1. It is seen that starting with an originally small negative temperature gradient in the mixture (1) a thermal runaway takes place leading to a steep reaction front. At the front, a pressure peak builds up and the velocity increases (2). When the front has travelled over 2 mm, the temperature and the pressure gradients have become very steep and the velocity peak is at 1000 m/s resembling that a detonation wave (3). This wave continues over the entire distance of 7 mm (4). Simulations of temperature gradient induced transition to detonation were recently performed by Ivanov et al. [9] for several hydrogen-oxygen mixtures. They clearly show the coupling between the reaction wave and the acoustic wave.

The novel aspect of the theory developed in [5],[6],[7] is the consideration of the original size of the ignition kernel as a measure for the region over which the temperature gradient must extend. This size appears in the context of a model of dynamic effects of auto-ignition kernels or ‘hot spots’ by Meyer and Oppenheim [10]. The model had been tested in numerical calculations by Lutz et al. [11] for a homogeneous mixture and shows how the mixture originally confined in a radius r_0 expands as the temperature increases due to homogeneous auto-ignition. Results of a numerical simulation using an elementary mechanism for iso-octane at 700 K initial temperature and 20 bar initial pressure p_0 based on the system of equations given in [11] are shown in figure 2. It is seen that after a relatively long induction time of 7.98 ms there occurs a first stage ignition with a small temperature

and pressure increase and a small increase of the normalized radius r/r_0 . Thereafter, a second stage ignition occurs at 8.35 ms where the temperature jumps to nearly 3000 K and the normalized radius increases to more than 4 times its initial value. The normalized pressure p/p_0 also shows a jump to 1.7 times its original value. This initiates sound waves which then may couple with the propagating reaction wave along a negative temperature gradient as predicted in [8]. Lutz et al. [11] have defined a so-called excitation time τ_e which is the time from the instant of 5% heat release rate to the maximum heat release rate. The normalized heat release Q/Q_{max} rate is shown in figure 2 on a logarithmic scale. At first stage ignition it is 1 % of the maximum value, then drops again to cross the threshold value of 5 % only at the time when both the pressure and the temperature rise very steeply. The time from there to the maximum heat release is extremely short and therefore cannot be shown in figure 2. Calculations show that it is typically three orders of magnitude smaller the ignition delay time and therefore of the order of microseconds. The product of the excitation time and the sound speed defines a length which corresponds to the distance the sound wave travels during the excitation time.

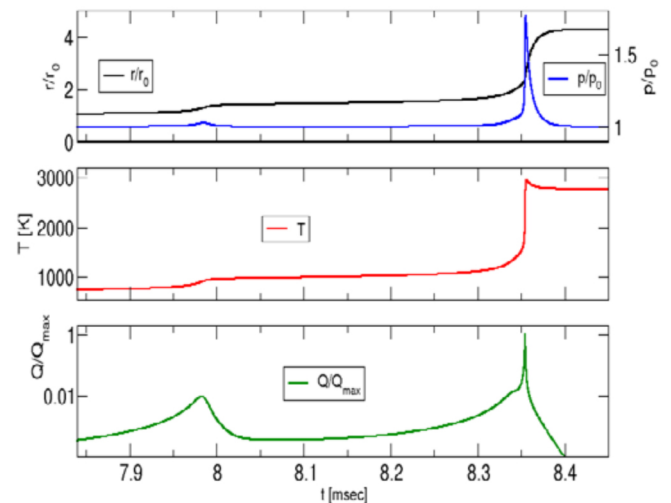


Figure 2. Auto-ignition of an ignition kernel of initial radius r_0 showing its increase due to temperature increase. The pressure increase at second stage auto-ignition and the heat release rate are also shown.

With the local temperature gradient $\partial T/\partial x$ assumed to be given, the reaction wave velocity can then be determined from eq. (1) and can be normalized by the sound speed at the local temperature to form a non-dimensional parameter

$$\xi = a/u = a * \partial T/\partial x * d\tau/dT.$$

(2)

In addition, the length of the region over which the temperature gradient is constant must be considered. If this length ℓ is equal or larger than the distance over which the sound wave emitted from the ignition kernel travels during

the excitation time, a resonance can be established. This condition defines another non-dimensional parameter ε as

$$\varepsilon = \ell / (a * \tau_e). \quad (3)$$

The two non-dimensional parameters have led the authors of [5],[6],[7] to define a regime diagram for developing detonations shown in [figure 3](#), in which the regime of a resonant developing detonation is located within limiting values of ξ , namely ξ_ℓ and ξ_u , which are a function of the value of ε .

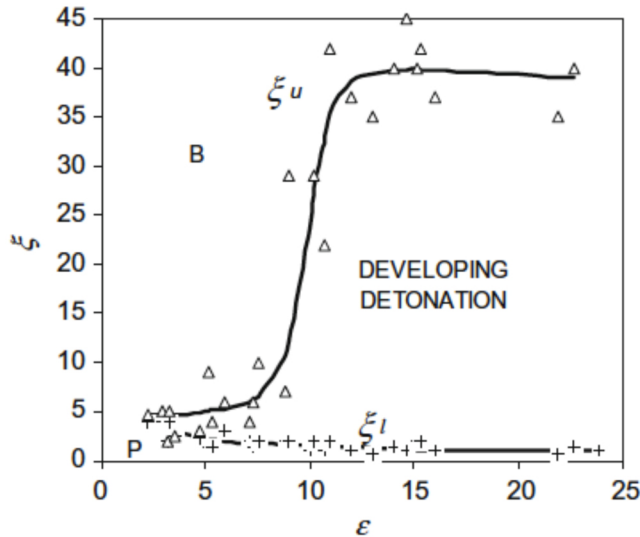


Figure 3. Regime diagram from [5] of the non-dimensional parameters ξ and ε defined in [eqs. \(2\) and \(3\)](#).

The region B in this diagram is the region $\xi > \xi_u$ which corresponds to subsonic deflagrations, the classical flame propagation mode. For $0 < \xi < \xi_\ell$ we have a super-sonic reaction wave propagation which therefore cannot couple with the sound speed. Finally, for $\xi = 0$ we have homogeneous auto-ignition. It is worth noting that for detonations to develop it is not necessary that the resonance condition $\xi = 1$ is satisfied exactly, but that there is a whole range of ξ - values between ξ_ℓ and ξ_u where this may happen.

The methodology developed in [5],[6],[7] has recently been applied by Rudloff et al. [12] to study pre-ignition events leading to cycles with low and high knock intensity in a single cylinder engine running at 1000 rpm with an IMEP of 27.4 bar. For a cycle of high knock intensity they note in the pressure trace two auto-ignition events where the second one would have caused violent pressure oscillations. They conclude, in agreement with the theory developed in [5],[6],[7], that the transition to a developing detonation depends mainly on thermodynamic conditions.

In principle, considering [eqs. \(2\) and \(3\)](#), the ignition delay time τ and its temperature dependence can be calculated as a function of temperature and pressure by using

a detailed kinetic mechanism for surrogate fuels representing gasoline. Based on such a mechanism also the excitation time τ_e can also be calculated by solving the system of equations given in [11].

On the other hand, the temperature gradient and the length over which it extends (characterized by the original size of the ignition kernel) has been guessed in the previous applications of the methodology. In [4], for instance, the temperature gradient was estimated as -1 K/mm or -2 K/mm and the original size of the ignition kernel as 5 mm. The latter was taken to be of the order of the integral length scale which can be estimated from the clearance height at TDC. However, under turbulent conditions, these quantities can only be statistical. Whether a smooth temperature gradient in the unburnt fuel-air mixture has the right order of magnitude over a sufficiently large spatial distance will require the knowledge of a joint distribution of the temperature gradient and of the length of monotonous temperature regions in the field. Clearly such regions are much smaller than the integral length scale. At the end of the compression stroke in a spark ignition engine, the temperature field is that of decaying turbulence with imposed mean velocity, temperature and equivalence ratio gradients. Although anisotropies persist on the large scales, the classical theory of turbulence predicts that at the small scales the field is essentially isotropic. However, the classical theory does not provide any information about the joint distribution requested here.

Only a refinement proposed by the first author and his group in recent years which is called dissipation element theory [13]-[14] is able to estimate the joint distribution of temperature gradients and of the length of the distance over which the temperature profile is monotonous. It is a theory focusing on the small scales of a scalar field. Dissipation elements are space-filling structures in a scalar field like the temperature, which can be constructed by using gradient trajectories. Starting from every point in the field a gradient trajectory in ascending direction will reach a maximum point, in descending direction it will reach a minimum point. A dissipation element is defined as the spatial region from which the same pair of maximum and minimum points is reached by gradient trajectories. Within that region therefore the scalar field is monotonous.

This is shown in [figure 4](#) which is extracted from a 2D-Direct Numerical Simulation (DNS) of homogeneous shear turbulence with an imposed mean scalar gradient [14]. The background field in this figure can be interpreted as that of the temperature in a turbulent flow. The blue colour indicates low values of the temperature and the yellow colour large values. Starting from any point in the field one may follow the steepest gradient in ascending and descending direction until one reaches a local maximum (red dots) or a minimum point (blue dots). The yellow lines represent the borderlines between dissipation elements. The figure shows that dissipation elements are space-filling objects which subdivide

the entire turbulent temperature field into smaller sub-units amenable to a more detailed analysis.

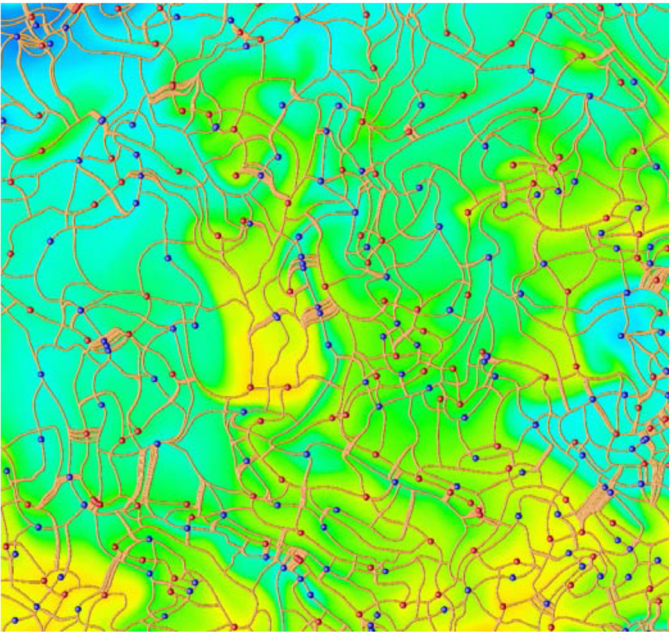


Figure 4. The figure shows the two-dimensional turbulent field of a passive scalar such as temperature in a turbulent flow, obtained from Direct Numerical Simulations. The scalar field is subdivided into so-called dissipation elements that are the ‘building blocks’ of a decomposition-reconstruction method for scalar fields [13]-[14]. The color marks scalar values ranging from maximum (yellow) to minimum (blue), red points are local maxima, blue points local minima, and yellow lines mark the border lines between the dissipation elements.

The cut-out shown in [figure 4](#) is approximately that of an integral length scale ℓ_t , the mean length scale ℓ_m of dissipation elements (the mean distance between a minimum and a maximum point) is approximately 2 Taylor length scales. This shows that the region covered by one integral scale is subdivided into many smooth regions of monotonous temperature. Only within those regions the acoustic resonance phenomenon between the reaction wave velocity and the sound speed can lead to a developing detonation which eventually can cause super-knock. To which extend variations of the temperature gradient within those region would modify this leading order statement needs to be examined. This would require further simulations of the kind performed in [6] using non-constant initial temperature gradients.

Let us consider the yellow region in the center of [figure 4](#) where two red maximum points appear. At a certain distance away from them appear a number of blue points indicating local minima. The temperature difference between a maximum and a minimum divided by the distance between them measures the mean temperature gradient in the dissipation element of which they are the ending points. In

the yellow region the following scenario can be imagined: During compression when the temperature increases auto-ignition may be initiated in the vicinity of the two red points. The yellow region therefore represents a ‘hot spot’ or ignition kernel as discussed in the context of [figure 2](#). We assume that the figure represents the situation at the end of the induction time when temperature changes are still negligible. During first stage ignition, but in particular during second stage ignition the exothermic reactions speed up such that the ‘hot spot’ is sending out strong acoustic waves in all directions. The ignition kernel has propagated by this time into the adjacent dissipation elements, and since these elements have a negative temperature gradient in direction of the reaction wave propagation, an acoustic coupling may take place. This could be imagined for the large element on the l.h.s. of the yellow region considered. Thereby a relatively large region (but still much smaller than the integral length scale) would detonate giving rise to high pressures as shown in [figure 1](#). At the end of this region, denoted by the blue minimum point on the upper left of the dissipation element considered, the temperature gradient changes sign and therefore the acoustic wave decouples from the reaction front. If the detonation wave is strong enough it will continue to propagate before it collapses. Even though the region where the high pressure develops is small and the time is short of the order of microseconds, the overall pressure rise may be large enough to accelerate the auto-ignition of larger regions and to lead to pre-ignition events or ‘super-knock’.

DETONATION PROBABILITY

We have performed 3D-DNS simulations of homogeneous isotropic turbulence, being the most generic case representing small scale turbulence, to obtain the statistics of the two parameters which characterize a dissipation element. The temperature difference between the values at the maximum and the minimum point is denoted by the parameter ΔT , the linear distance between the points is denoted as the parameter ℓ . The joint probability density function $P(\ell, \Delta T)$ of these two parameters normalized by their mean values ΔT_m and ℓ_m , respectively, is shown in [figure 5](#).

It can be converted into a normalized joint pdf of the gradient $g = \Delta T / \ell$ and ℓ . Here g denotes the mean gradient of the temperature along a dissipation element and therefore approximates the local temperature gradient within a dissipation element. Together with its length ℓ we therefore know the joint probability density of the temperature gradient and the length over which it extends in the turbulent temperature field. The normalized joint pdf $P(\ell, g)$ is shown in [fig. 6](#). In [13] a model equation has been derived for the marginal distribution of the length ℓ . This distribution decays exponentially for large values of ℓ .