

Impact of Particle Characteristics and Engine Conditions on Deposit-Induced Pre-Ignition and Superknock in Turbocharged Gasoline Engines

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ABSTRACT

Low Speed Pre-Ignition (LSPI), also referred to as superknock or mega-knock is an undesirable turbocharged engine combustion phenomenon limiting fuel economy, drivability, emissions and durability performance. Numerous researchers have previously reported that the frequency of Superknock is sensitive to engine oil and fuel composition as well as engine conditions in controlled laboratory and engine-based studies. Recent studies by Toyota and Tsinghua University have demonstrated that controlled induction of particles into the combustion chamber can induce pre-ignition and superknock. Afton and Tsinghua recently developed a multi-physics approach which was able to realistically model all of the elementary processes known to be involved in deposit induced pre-ignition. The approach was able to successfully simulate deposit induced pre-ignition at conditions where the phenomenon has been experimentally observed. This approach allowed characterization of the impact of particle characteristics, bulk charge properties and engine conditions and provided valuable insight into behavior observed in engine and bench tests.

The objective of this study is to develop a conceptual model for deposit-induced pre-ignition based on first principles, and to provide the industry a framework to help model this complex phenomenon and to help guide optimization of engine design, control and fuel and lubricant compositions for real world LSPI suppression. In this work, multi-physics simulations were conducted that incorporated accurate representation of heat and mass transfer, particle oxidation and gas-phase autoignition and specific characteristics of the particle that dominate pre-ignition were identified. The study was extended to simulate the effect of bulk charge properties and engine conditions on pre-ignition. The results show that pre-ignition timing, and therefore superknock, is particularly sensitive to key deposit characteristics and engine operating conditions, consistent with results of experimental studies that have been reported in literature. The results of this study help elucidate the phenomenon of deposit induced pre-ignition that has been reported but is not well understood. Furthermore, the results of this study will aid the industry in development of improved fluid formulations and engine design that are needed to suppress superknock in real-world turbocharged engines.

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INTRODUCTION

Low Speed Pre-Ignition (LSPI), also referred to as super-knock or mega-knock, is an undesirable phenomenon observed in turbocharged gasoline engines, particularly at low-speed and high-load conditions. This phenomenon potentially limits the robustness of modern engines. Furthermore, engine control strategies or other mechanical measures implemented to mitigate LSPI in turn limit the fuel economy, power, emissions and drivability gains that otherwise may be realized through adoption of boosted and downsized engine technologies. Wang and coworkers have published an excellent review of the recent progress in understanding the fundamentals of conventional knock and superknock [1].

Even though pre-ignition was reported in boosted gasoline engines as early as 2007 [2], and been the subject of a large number of studies [3, 4, 5, 6, 7, 8, 9], the dominant mechanism for LSPI in production engines has not been conclusively identified - which attests to the fact that LSPI is triggered by a complex mechanism that is still not fully understood. Without a complete understanding of the underlying mechanism, the industry is forced to deploy more empirical approaches at a considerable effort and involving significant trade-offs as noted above. We believe that taking a fundamental, science-based approach to understanding the mechanism behind pre-ignition is necessary to develop robust, real-world solutions.

Two possible mechanisms for pre-ignition have been proposed to explain the stochastic nature of pre-ignition. Oil-fuel droplets ejected from the piston crevice [3,5,6,10,11,12,13] and combustion

chamber deposits [4,14,15]. In a recent study, Afton applied a systematic approach to deconvolute the mechanism of droplet-induced pre-ignition into elementary steps [10]. Based on the elementary steps, a 3D CFD simulation was developed, which was able to predict droplet induced pre-ignition successfully, and was used to predict the effect of injection timing on pre-ignition timing. The predictions were in good agreement with experimental observations, and were able to explain the non-linear relationship between injection and pre-ignition timing as well as the key fluid properties that drive pre-ignition behavior at real world conditions.

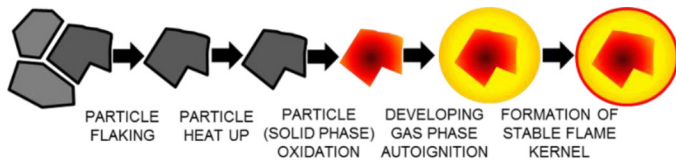


Figure 1. Conceptual model for deposit induced pre-ignition

In the present study, a conceptual model (shown in Fig 1 above) is proposed for the deposit induced mechanism, which proceeds through sequential elementary steps that are expected to take place for successful pre-ignition of the fuel/air mixture at engine conditions. A systematic approach of deconvoluting the deposit induced pre-ignition mechanism into its elementary steps allows the development of realistic multi-physics simulations that are able to incorporate quantitative representation of the elementary processes. The results of the simulations are consistent with recent experimental studies conducted on a well-controlled research engine [14] and with experimental studies conducted on production engines [3, 6, 7 and 9]. A simulation based approach is able to help explain the effect of the deposit characteristics and engine conditions on pre-ignition, something extremely challenging to achieve experimentally, considering the time and length-scales involved in engine combustion.

RECENT EXPERIMENTAL STUDIES

Despite significant circumstantial evidence, such as visualization using high speed in-cylinder imaging [15] supporting deposit induced pre-ignition, relatively few studies have reported on the deposit induced pre-ignition mechanism.

Deposit formation on combustion chamber surfaces is a complex process that has been studied by a number of researchers [16, 17, 18]. This process is known to be sensitive to a range of parameters, such as fuel and lubricant composition and volatility, as well as surface temperatures [17] and engine operating conditions [19]. The composition of the combustion chamber deposits, and therefore the particles expected to flake off is predominantly carbonaceous, though inorganic material is often present [20-21].

Despite the stochastic nature of the process, as well as the challenges involved in measuring such a phenomenon, combustion deposit flaking has been reported in literature. Kalghatgi and coworkers have published a number of studies on combustion deposit flaking [22, 23, 24]. The mechanism of deposit flaking is not well understood, but has been reported to be sensitive to fuel composition and humidity [24].

More recently, visualization of in-cylinder processes through high speed photography has indicated that violent superknock presumably dislodges particles from combustion surfaces.

Due to the complexities involved with testing the effect of deposits using production engines, as well as lack of control on size, concentration and composition, only a very limited number of studies have been conducted on deposit induced pre-ignition using production engines. To improve control of deposit size, concentration and composition, some studies have used controlled injection of particles as a way to approach the problem.

Okada and coworkers at Toyota [15] studied LSPI in a turbocharged GDI engine and used visualization to identify the presence of particles in the combustion chamber using a high speed camera and an artificial light source for illumination. In-cylinder pressure was simultaneously recorded to identify timing of start of combustion and therefore pre-ignition. Images taken from the high speed camera were reported that showed the presence of material in the combustion chamber, potentially deposits. Flame fronts were observed to initiate close to the spatial location of these particles. Cycles for which particles were observed also indicated pre-ignition based on in-cylinder pressure data. In the same study, Okada and coworkers also investigated pre-ignition through controlled injection of particles into the intake manifold. A range of material was injected and evaluated for LSPI, and the inability of non-combustible material (calcium sulfate, sodium chloride and cigarette ash) to induce pre-ignition was reported. Inability of carbon black and soot extracted from exhaust pipe to induce pre-ignition was also reported, and ascribed to small particle size (reported to be about 20 to 100 nm). Combustible materials, namely cigarette leaf, instant coffee, milled coffee beans and deposits taken from the combustion chamber were able to induce LSPI. The range of timing of start of combustion induced by pre-ignition by these materials appeared to be similar to the range of timing of start of combustion for naturally occurring pre-ignition.

Wang and coworkers at Tsinghua University [14] studied the effect of particle characteristics on pre-ignition in a single cylinder research engine through controlled injection of carbon particles. This approach offered an improved platform compared to production engines, where control of deposit size and temperature is not possible. The study found that higher particle temperature led to earlier pre-ignition and superknock. Increased particle size also led to earlier pre-ignition. The relatively well-controlled conditions used in the study and the well-characterized properties of activated carbon used in literature allow a good study for simulation and model validation.

CONCEPTUAL MODEL OF DEPOSIT INDUCED PRE-IGNITION

The conceptual model (shown in Fig 1 above) depicts the deposit induced mechanism through sequential elementary steps that are expected to take place for successful pre-ignition of the fuel/air mixture at engine conditions. The specific elementary steps leading to formation and growth of the premixed flame kernel are summarized below.

1. Particle dislodgement/flaking from combustion chamber surfaces or *in-situ* formation from unvaporized droplets
2. Particle heat-up
3. Particle (solid phase) oxidation
4. Local auto-ignition driven by gas-phase kinetics
5. Formation of stable and growing flame kernel

The conceptual model proposed here provides a framework from which a predictive pre-ignition simulation based on particle characteristics and engine conditions could be developed. By modeling the elementary steps, a multi-physics simulation, capable of capturing the interaction between different and simultaneous processes could be captured. Further details of the simulation are presented in the following section.

SIMULATION DEVELOPMENT

Particle Heat Transfer

To model the solid particle thermal characteristics and heat transfer between it and the surrounding gas, we make several assumptions for simplicity.

The model assumes:

- The particle is spherical, and its temperature only varies radially.
- Convection is the dominant mode of heat transfer (radiative heat transfer is negligible)
- Constant bulk properties (independent of radius, temperature and time)
- The thermal inertia of the particle is small compared to the bulk gas, so bulk gas temperature is independent of particle temperature and does not vary spatially

The rate of heat transfer between a sphere and the fluid surrounding it could be limited by rate thermal conduction within the sphere (internal heat transfer) or the heat transfer between the surface of the sphere and the fluid (external). The Biot number, a dimensionless number, can help identify which one of these effectively limits the overall rate of heat transfer. The Biot number for a sphere is expressed as:

$$Bi = \frac{h * L}{k}$$

where h is the heat transfer coefficient, L is the characteristic length scale and k is the thermal conductivity.

Using the heat transfer coefficient calculated based on engine conditions, thermal conductivity of carbon and the radius of the particle to represent the effective length scale, the Biot number can be calculated. For the conditions predicted by the simulations, the Biot number was found to be relatively small. This suggests that considering the relatively small size of the particles, the conduction (solid phase heat transfer) is relatively quick compared to the heat transfer across the solid-gas interface. Therefore the heat transfer coefficient can be used to represent the overall rate of heat transfer,

and radial variations in particle temperature can be neglected. Details on the appropriate calculations for estimation of heat transfer for a sphere in an infinite medium can be found in [25] and [26]. The effect of heat generation due to particle oxidation was also taken into account (details described below).

Fig. 2 below depicts the local flowfield in the proximity of the particle at engine conditions. The Reynolds number was calculated to help characterize the local flow behavior and help guide the estimation of the effective heat transfer coefficients between the particle and the bulk gas. Considering the small particle size, relatively very small Reynolds numbers are predicted. This suggests that the local flowfield will be laminar, often characterized as 'creeping flow'. At such flow regimes, the heat transfer approaches a condition where conduction becomes the dominant mode of heat transfer, and helps estimate an asymptotic value of the heat transfer coefficient which can then be implemented in the model. As the rate of heat transfer between the particle and the boundary layer is expected to be relatively fast compared to the heat transfer between the boundary layer and the bulk gas, the temperature of the boundary layer is assumed to be close to the particle temperature. The rate of heat transfer between the boundary layer and the bulk gas can then be represented using a heat transfer coefficient. Considering that the temperature of the gas in the boundary layer and wake of a hot particle is expected to have a higher temperature than the bulk gas, the boundary layer and wake region will be the most likely location for pre-ignition. Therefore the temperature of the boundary layer can be used to predict the gas-phase autoignition kinetics (described below). The various zones (particle, boundary layer and bulk) considered in the particle heat transfer model and their respective temperatures are indicated in Fig. 2 below.

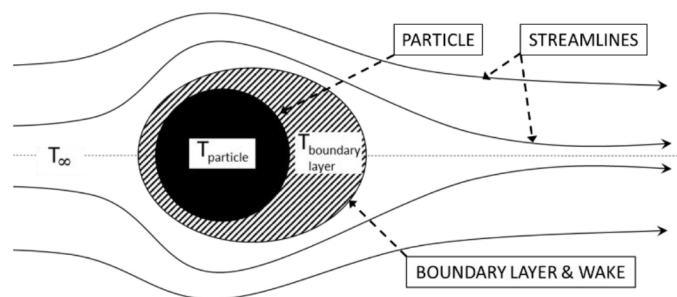


Figure 2. Depiction of streamlines expected at the low Reynolds number conditions representative of local flowfield in the proximity of the particle at engine conditions. The various zones (particle, boundary layer and bulk) considered in the particle heat transfer model and their respective temperatures are indicated.

Particle Mass Transfer

Considering the bulk gas temperatures predicted at engine conditions, the kinetics of solid-phase oxidation are expected to be sufficiently high to lead to significant rates of oxidation. Considering the relatively small size of the particles, the burn-off, and reduction in size of the particles cannot be neglected, as it will subsequently affect properties like thermal inertia and heat transfer. Based on the rates of oxidation predicted by the kinetic model, the rate of mass of carbon was calculated, and based on the spherical particle assumption, an effective rate of reduction in radius was calculated at each time-step.

Bulk Fuel-Air Mixture Conditions

Bulk charge properties were estimated for the engine used by Tsinghua in their experimental study [14], and specific engine parameters used for the simulation are shown in Table 1 below. The average charge temperature and pressure were calculated as a function of crank angle based on the slider crank mechanism. A polytropic coefficient of 1.37 was used in the calculations for the compression and power stroke. Intake Valve Closing (IVC) was fixed at -140 aTDC. Further details on the experimental setup and fuel properties can be found in [14].

Table 1. Engine specifications and operating conditions used for simulations, based on [14]

Cylinder	1
Displaced volume	0.815 L
Stroke	115 mm
Bore	95 mm
Compression ratio	14:1
Manifold Air Pressure	0.1 MPa
Engine Speed	1200 RPM
Fuel	Gasoline (Port Fuel Injected)
Air-Fuel Ratio	Stoichiometric
Intake Air Temperature	20°C

Solid-Phase Oxidation Kinetics

Kinetics for oxidation of the carbon particles have been taken from the work of Miyamoto and coworkers [27]. Measurements of the rate of oxidation of carbon particles was conducted for the present study using thermogravimetric analysis for comparison with the values reported by Miyamoto and coworkers, and the results were found to be in excellent agreement. The kinetics of Miyamoto and coworkers are also consistent with those published by several different studies for a wide range of temperatures and experimental techniques, and a comparison can be found in [28].

Gas-Phase Autoignition Kinetics - Pre-Ignition Integral

Livengood and Wu [29] presented an elegant and convenient approach to predicting autoignition for gasoline-air mixtures by representing the ignition delay ' τ ' of a mixture as an Arrhenius expression (as a function of pressure ' p ', temperature ' T ', and coefficients ' A ', ' n ' and ' B ')

$$\tau = A p^{-n} \exp (B/T)$$

Through this approach, the sensitivity of ignition delay to temperature and pressure could be represented. To predict the timing of ignition delay of a mixture undergoing a process with varying conditions of pressure and temperature, such as in engine combustion, Livengood and Wu proposed a parameter ' ϕ ' that represented the inverse of the ignition delay τ at a particular temperature and pressure:

$$\phi = \frac{1}{\tau}$$

Considering the path of temperature and pressure followed by the ignitable mixture, ϕ can be integrated as a function of time. The time at which the integral equals unity is the predicted ignition timing. This approach offers a convenient method to predict the ignition delay in engines, where temperature and pressure as a function of crank angle can be calculated from engine parameters:

$$\int_{t=t_0}^{t=t_{\text{ignition}}} \phi dt = 1$$

This approach was further improved by Douaud and Eyzat [30], who extended and validated this approach to commercial gasoline fuels. They proposed expressions in their study that allowed prediction of ignition delay based on the octane number of the fuel.

This approach was used in the present study to predict pre-ignition. Using this approach, the Pre-ignition Integral is calculated at each crank angle based on the pressure in the combustion chamber and the temperature of the boundary layer and wake zone at that crank angle. The pre-ignition timing for the simulation can be identified for the crank angle at which the Pre-ignition Integral reaches a value of 1 - a very convenient method to compare predictions with experimental observations.

Deposit Physical and Thermal Properties

Since properties of activated carbon were not provided in [14], properties were taken from peer-reviewed publications. To ensure self-consistency, publications reporting multiple properties were preferred. Henning and coworkers [31] report a number of properties of coal derived activated carbon, and was used as the source of most of the properties used for the simulations. A density of 600 kg/m³, specific surface area of 400m²/g and a heat capacity of 850 J/kg.K is reported by [31] and was used for the simulations. A heat of combustion of 34.08 kJ/kg is reported by [32] and was used in the simulations.

RESULTS: EFFECTS OF DEPOSIT CHARACTERISTICS

Tsinghua [14] recently studied the effect of initial particle temperature on pre-ignition, and found that for a particle temperature of 25°C, no pre-ignition was observed, though pre-ignition was observed for initial particle temperatures of 300°C, 370°C and 450°C. Simulations were conducted using the engine conditions reported in [14] to predict the particle temperature histories, as well as the pre-ignition integrals, and are shown in Fig. 3 below.

The predictions of particle temperature and pre-ignition integral for the three different initial particle temperatures is shown in Fig. 3 above. Through the intake stroke and early part of the compression stroke, the particle temperatures drop, consistent with the heat transfer to the much cooler fuel-air mixture for an intake air temperature of 20°C. After IVC at -140° aTDC, polytropic