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PREDICTING SUPER-KNOCK IN IC ENGINES USING MACHINE LEARNING

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Abstract. We investigate the prediction of super-knock in internal combustion (IC) engines by using machine learning (ML). The dataset generated from multi-dimensional direct numerical simulations (DNS) of knock formation for a stoichiometric ethanol/air mixture under a representative end-gas auto-ignition condition in IC engines is adopted to train a Deep Neural Network and assess its predictive capability.

Highly boosted and downsized engine strategies have been widely investigated for advanced engines. The engines become more compact, and thus provide higher power density per volume, higher thermal efficiency, and lower CO_2, NO_x and soot emissions. Despite their promising advantages over the conventional IC engines, the elevated pressure and temperature of the in-cylinder fuel/air mixture under high-load operating conditions may induce a higher propensity of abnormal combustion phenomena such as pre-ignition, knock, and even super-knock [1, 2, 3]. Such abnormal combustion phenomena also occur in shock tubes, rapid compression machines, and gas turbine engines [3]. Super-knock is characterized by extremely high-pressure spikes and excessive pressure oscillations that may lead to mechanical damage [3]. The better understanding of the underlying mechanism of the super-knock development and a reliable criterion to predict super-knock are needed to prevent destructive operation of combustion devices [4, 5, 6].

First-principle direct numerical simulations (DNS) can fully resolve all temporal and spatial scales and the complex interaction of thermochemistry and turbulence [1, 2]. Such high fidelity simulations allow unraveling the process of detonation development encountered in advanced combustion devices under extreme high-load operating conditions as illustrated in Fig. 1. With the aid of machine learning and high-fidelity DNS data, a

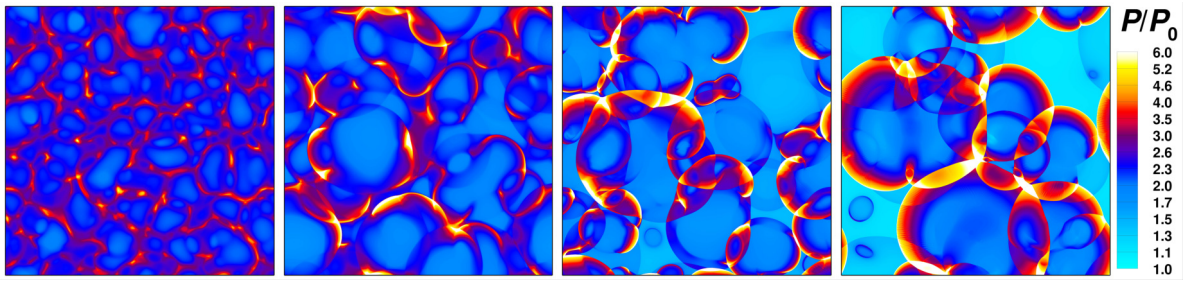


Figure 1: Representative distribution of pressure for four different l_e of 1 mm, 2 mm, 5 mm, and 10 mm from left to right, with the same T' of 15 K. Cases with l_e of 1 mm, 2 mm, and 5 mm and 10 mm, feature no knock, mild knock, and super-knock, respectively.

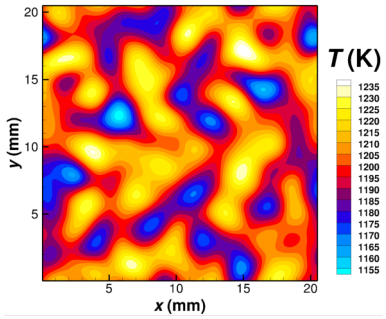
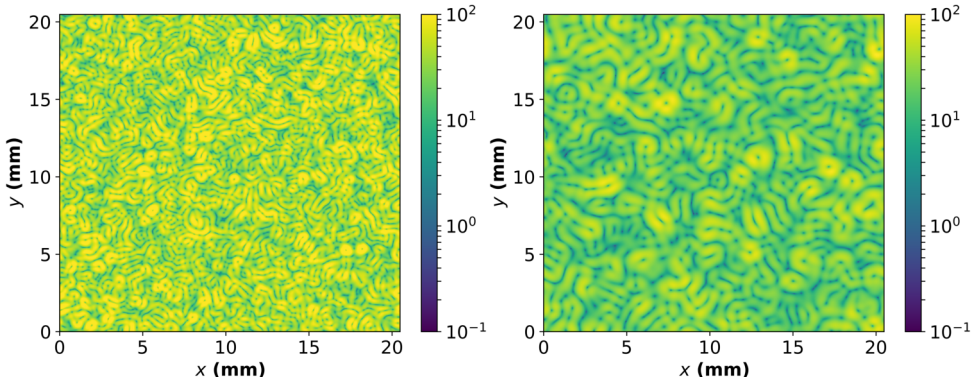


Figure 2: Representative distribution of temperature with T' of 15 K for l_e of 5 mm. T' and l_e denote the root mean square temperature fluctuation, and the most energetic length scale of temperature, respectively.

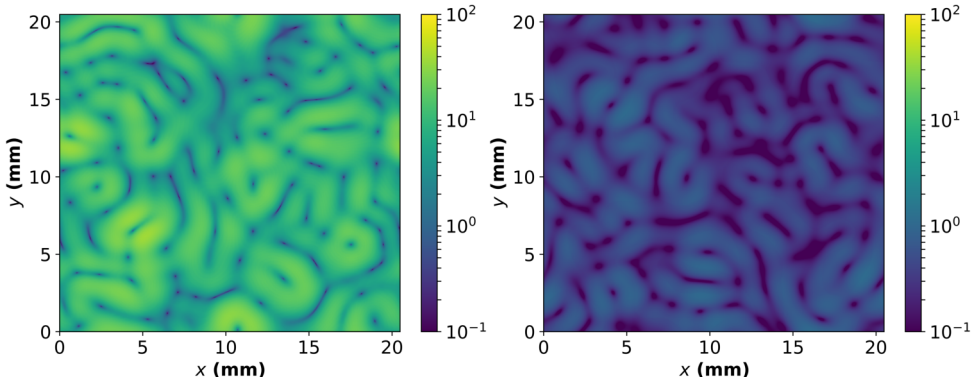
framework to predict the knock propensity for a given initial condition is being developed, which can serve as a reliable predictive tool for real-world industrial applications.

The dataset to apply machine learning was generated in previous parametric DNS studies [1, 2]. The possibility of super-knock events is predicted for given initial conditions as those representatively shown in Fig. 2 and Fig. 3, and the temporal and spatial evolution of the flow field. The initial conditions correspond to a temperature T_0 of 1200 K, pressure P_0 of 35 atm, and equivalence ratio ϕ_0 of 1.0. Under these initial conditions, the associated homogeneous ignition delay time, τ_{ig}^0, and equilibrium pressure, P_e, of the ethanol/air mixture are 75 μs, and 99 atm, respectively. Other relevant ideal one-dimensional detonation parameters are the von-Neumann pressure, P_{VN} of 315 atm, Chapman–Jouguet pressure, P_{CJ} of 185 atm, and Chapman–Jouguet speed, V_{CJ} of 1836 m/s. Further details will be provided in the presentation.

Deep learning is a class of machine learning tools based on artificial neural networks with representation learning. Deep learning has been successfully applied in various fields including industrial automation[7], cloud computing [8], and medicine [9]. However, its applications in computational fluid dynamics (CFD) workflows are sparse [10]. In the current work we employ a deep learning technique to predict super-knock. A deep neural



(a) $l_e = 1$ mm, $T' = 15$ K, no knock (b) $l_e = 2$ mm, $T' = 15$ K, mild knock



(c) $l_e = 5$ mm, $T' = 15$ K, super-knock (d) $l_e = 5$ mm, $T' = 0.6$ K, mild knock

Figure 3: Representative ξ distribution computed from the initial conditions for three different l_e of 1 mm, 2 mm, 5 mm from left to right, with the same T' of 15 K.

network (VGG16) is trained to predict three cases including no-knock, mild-knock and super-knock. The trained network is evaluated using manually labelled data. Such an approach will be used for inference, i.e. with a given initial conditions shown in Fig. 2, we are able to predict if there is a super-knock event or not. Such a capability will save computational resources in the order of millions of core hours.

The prediction is based on the spatial distribution of ξ [4], which is defined as $\xi = a/S_{sp}$, where S_{sp} is the speed of a spontaneous ignition front and defined by the spatial gradient of the ignition delay time, $S_{sp} = |\nabla \tau_{ig}|^{-1}$, and a is the sound speed. The initial conditions of seventy eight cases featuring different knock levels were processed, resulting in the seventy eight distributions of ξ as shown in Fig. 3. The data were divided into training and testing splits, 62 images were used for training and 16 were used for testing. All data were classified into three classes - no knock, mild knock, and super-knock. In order to feed unbiased data to the network, training and testing data had proportional representation of data from all classes.

The trained VGG16 network was able to predict test data with very high accuracy, almost 100% in many cases. This deep learning technique also confirmed a strong correlation

between the knock intensity and the level of root-mean-square temperature fluctuation, T', and its characteristic length scale, l_e. In future we will be conducting more deeper studies and we will pose more harder questions such as the identification of localized super-knock regions and early prediction of super-knock.

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