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LES of knocking in engines using dual heat transfer and two-step reduced schemes

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ABSTRACT

Large Eddy Simulation of knocking in piston engines requires high-fidelity physical models and numerical techniques. The need to capture temperature fields with high precision to predict autoignition is an additional critical constraint compared to existing LES in engines. The present work presents advances for LES of knocking in two fields: (1) a Conjugate Heat Transfer (CHT) technique is implemented to compute the flow within the engine over successive cycles with LES together with the temperature field within the cylinder head walls and the valves and (2) a reduced two-step scheme is used to predict both propagating premixed flames as well as autoignition times over a wide range of equivalence ratios, pressures and temperatures. The paper focuses on CHT which is critical for knocking because the gas temperature field is controlled by the wall temperature field and knocking is sensitive to small temperature changes. The CHT LES is compared to classical LES where the temperatures of the head and the valves are supposed to be homogeneous and imposed empirically. Results show that the skin temperature field (which is a result of the CHT LES while it is a user input for classical LES) is complex and controls knocking events. While the results of the CHT LES are obviously better because they suppress a large part of the empirical specification of the wall temperatures, this study also reveals a difficult and crucial element of the CHT approach: the description of exhaust valves cooling which are in contact with the engine head for part of the cycle and not in the rest of the cycle, leading to difficulties for heat transfer descriptions between valves and head. The CHT method is successfully applied to an engine studied at IFP Energies Nouvelles where knocking characteristics have been studied over a wide range of conditions.

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1. Introduction

To increase the efficiency of reciprocating engines, downsizing has become a new standard in the automotive industry [1]. By combining smaller cylinder sizes with turbo-chargers, engines can be operated in a region of higher efficiency. For moderate downsizing levels, this technique enables to decrease fuel consumption significantly and thus pollutants emissions. However abnormal combustions prevent engine manufacturers from using advanced levels of downsizing. Abnormal combustion results from the competition between the turbulent propagation of the premixed flame initiated by the spark plug and the spontaneous ignition of the fresh gas. When high pressure and high temperature are encountered in the fresh gas in front of the flame front (also called end-gas), the auto-ignition delay drops and can become lower than the time needed by the premixed flame to burn the charge. This kind of auto-ignition events leads to abnormal combustions such as knocking or rumble and can destroy the engine. Over the last decades, the increase of engines compression ratios lead to the same issues [2,3] and a better understanding of heat transfer and engine cooling allowed to control knocking. Nowadays, such fluid/solid interactions remain a key-parameter but it is not sufficient to control abnormal combustions in highly downsized engines. Increasing the engine resistance to knocking requires a better understanding of these phenomena. Although optical diagnostics are not easy to perform, existing experimental studies [4–6] highlighted some key features leading to abnormal combustions: (1) the intensity of knock is linked to the portion of fresh gas when auto-ignition occurs [7] and (2) detonation waves may appear in knocking cycles. The basic mechanism leading to detonation in such flows was studied by Zeldovich [8] who showed that a 1D temperature gradient in a flow close to auto-ignition could initiate a detonation wave. This mechanism was studied later by Bradley et al. [9] or Clavin et al. [10] and

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Table 1
Properties of the materials used in the CHT simulation.

	Symbol	Cast iron	steel
Density [kgm^{-3}]	ρ	2675	7500
Heat capacity [J/(kg K)]	Cp	900	450
Heat conductivity [W/(m K)]	λ	100	36

has become the prototype configuration used to illustrate how detonation can begin in an engine. Even though detonation can hardly be observed directly inside a piston engine several studies were carried-out in canonical configurations [8,11] suggesting that conditions were indeed favorable to detonation in knocking engines.

In this context, Large Eddy Simulations (LES) can provide detailed information to analyze abnormal combustion. Peters et al. [12] used simulations to identify regions where a Deflagration to Detonation Transition (DDT) can occur based on cold flow LES results and on the Zeldovich et al. theory. Robert et al. [13] proved that LES can be used to evaluate the knocking tendency of an experimental engine. They retrieved quantitatively the experimental behavior of the real engine and performed a first analysis of abnormal combustion thanks to LES.

Obviously temperature plays a major role for knock and in a real engine the temperature field is expected to control knocking events to a large extent. For instance, wall heat transfer dictates the temperature level at Top Dead Center (TDC) when ignition is performed just before knock can begin near hot regions. This issue becomes even more important for engines running with abnormal combustion where local and intermittent hot spots found near high temperature walls can initiate auto-ignition inside fresh gases. In that sense, the use of realistic wall temperatures is of first importance when studying abnormal combustions with numerical simulations. The potential benefits of conjugate heat transfer simulations for piston engines flows are pointed out in [14] and the same methodology is used in [15]. These studies proved that abnormal combustion events are influenced by wall temperatures and that Conjugate Heat Transfer (CHT) must be accounted for in these simulations, even in the context of RANS simulations. Here, the impact of CHT on knocking is investigated using individual cycles computed with LES. The drawback of this method is that hundreds of cycles would be needed to account for cycle to cycle variabilities and obtain converged statistics, thus implying large CPU cost and simulation times. In this context, recent LES work [16–18] proved that, with a limited number of cycles, LES can predict cyclic variations. More recently, it was also shown that LES can provide detailed informations on knocking with a few engine cycles only [13]. The scope of the present paper is to improve abnormal combustion LES by including a comprehensive description of conjugate heat transfer with LES.

2. Configuration and methodology

In an engine, conjugate heat transfer controls wall temperatures and has a strong impact on combustion [19] because of the long residence time of the fresh gas in the cylinder prior to combustion triggered around TDC. The large variations of the combustion chamber volume and thus of the thermodynamic conditions promote heat exchanges at the boundaries and impact the combustion process. The wall temperatures used in numerical simulations are usually obtained from experimental measurements or from *a priori* estimations. This approach can provide an appropriate global behavior but local information is missing. In particular, the sophisticated cooling system used for the cylinder head can lead to temperature in-homogeneities that can have an impact on abnormal combustion. Only one hot wall zone can be enough to trigger knocking. This situation differs from ‘classical’ LES in engines, far from knocking conditions where wall temperatures play a more limited role [20–22]. In this paper, conjugate heat transfer is solved by means of a fully coupled simulation between fluid and solid so that relevant boundary conditions can be used to study knocking. While such studies have already been performed using RANS [15], they require much more care in a true LES framework as described in the next section.

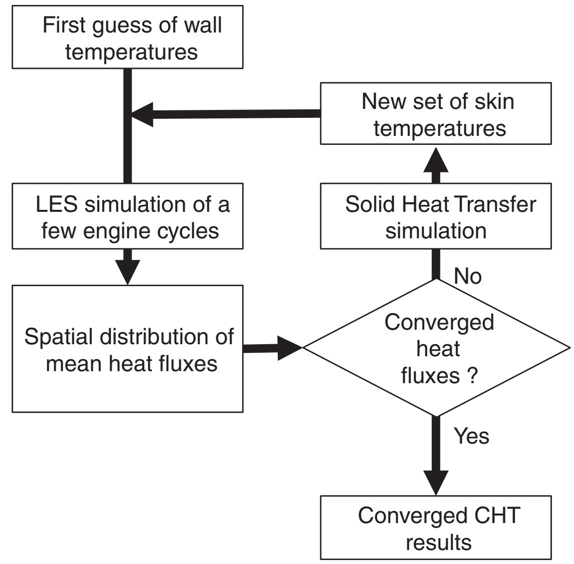

Fig. 1. Diagram of the weak coupling algorithm to perform a CHT simulation.

2.1. Coupling methodology

In order to use realistic boundary conditions, a common strategy consists in using two different solvers: one for LES and another one to solve the heat equation in the solid domain. In such simulations, the characteristic time of the heat conduction in the solid $\tau_s \sim L^2/D_s$ (with L the solid characteristic length and D_s the solid diffusivity) is often several orders of magnitude higher than the combustion characteristic time $\tau_c \sim \delta_l/S_L$ (with δ_l the flame thickness and S_L the flame speed). For instance, assuming a valve head of $L = 10$ mm and with the properties of steel (Table 1), the conduction characteristic time is:

$$\tau_s = \frac{L^2}{\lambda/(\rho Cp)} = \frac{0.01^2}{36/(7500.450)} = 9\,\mathrm{s} \quad (1)$$

while for an iso-octane/air flame at 40 bar and 700 K, the combustion characteristic time is:

$$\tau_c = \delta_l/S_L = \frac{1.10^{-4}}{1.0} = 1.10^{-4}\,\mathrm{s} \quad (2)$$

For this particular case, the conduction characteristic time is five orders of magnitude bigger than the conduction characteristic time: the solid acts like a low-pass filter and only sees a mean heat flux coming from the fluid domain. A numerical difficulty directly introduced by this time scales difference is that the convergence speeds differs in the fluid and in the solid domains. The convergence for the solid temperature is too long to be computed with LES. In practice however, this time scales difference can be exploited efficiently by recognizing that only a weak coupling between the two domains is sufficient. Decoupling the computations of LES in the cylinder and temperature in the solid walls allows to reach a converged state at the fluid/solid interface by only considering a mean averaged field of heat fluxes as inputs for the heat transfer simulation in the solid. The methodology used to obtain the converged conjugated heat transfer at the fluid/solid interface is based on such a weak coupling (Fig. 1). The two solvers are run sequentially: first, an initial set of wall skin temperatures is obtained from experimental measurements or from 0D

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