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DNS IGNITION OF OXYGENATED AND CONVENTIONAL HYDROCARBON FUELS IN A NON-HOMOGENEOUS TURBULENT FIELD WITH HIGH DISSIPATION RATE

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ABSTRACT

The present paper employs Direct Numerical Simulations (DNS) to gain insight into the early ignition process in a non-homogeneous turbulent flow where cool fumigated fuel is mixing with hot air. The two fuels considered are a model for oxygenated fuel (DiMethyl-Ether - DME) and a model for conventional hydrocarbon fuel (n-heptane). The non-homogeneities in temperature lead to changes in comparative ignition times between DME and n-heptane, as the latter burns on the hot air side because of a lower stoichiometry. Subtle effects of micro-mixing are thus able to modify the combustion phasing in compression-ignition mode and this study highlights the need for accurate ignition models in turbulent inhomogeneous mixtures.

INTRODUCTION

The main characteristic of biofuels is the presence of one or several oxygen atoms in the fuel molecule. The major impact is the reduction of the heat power per unit of mass. On the other hand, less oxidizer is necessary to burn a unit mass of an oxygenated fuel. This compensates the reduced heating value of the fuel and a flame temperature typical of hydrocarbons is preserved while more oxygen is available, likely to favour Zeld'ovitch NO_x . As NO_x are acknowledged to be produced early in the combustion process in an engine, the quality of ignition is a key to emission control. A better understanding of the ignition process of oxygenated fuels compared to conventional hydrocarbons is thus of significant importance.

With new computing resources, DNS of ignition in generic turbulent flows incorporating complex chemistry become increasingly popular. Hydrogen remains a fuel of preference given the modest complexity of its chemistry: [1-4]. Recently, a two-phase DNS of n-heptane ignition has been carried out [5,6]. Another one has been achieved using a reduced mechanism in the framework of a mixing layer [7].

The objective of the paper is to make use of the unique capabilities of DNS to gain insight into the processes of ignition in a non-homogeneous turbulent flow of an oxygenated fuel compared to a conventional hydrocarbon. Two representative fuels are employed for this purpose: DiMethyl-Ether (DME - for oxygenated fuel) and n-heptane (for normal alkane). The method, model problem and configuration are described in the following section. Preliminary results from this on-going research are discussed thereafter.

MODEL PROBLEM

The chosen configuration is a 257^2 2-D square box for computational ease (but it is known that the complex turbulent energy cascade is a 3-D process – this is one of the limitations of the presented simulations) in which the initial fields are carefully defined. The turbulence (velocity and pressure) is imposed in term of integral length \mathcal{L} and root-mean-square velocity u' while the scalar field is imposed through mean fuel mass fraction mixed with air and segregation factor ($\sigma = Y'_F / Y_F / (I - Y_F)$ in usual notations). A crude mixing law in temperature is built based on the relative concentration of fuel and air and their respective temperatures. This law of mixing approximates to the first order the temperature fluctuations due to fuel fumigation in air. Those are the expected local heterogeneities in a combustion chamber far from boundaries [8,9]

The spectrum model is the Passot-Pouquet formalism, [10], for a 2-D homogeneous turbulent field:

$$E(k) = \frac{32}{3} \sqrt{\frac{2}{\pi}} \frac{u'^2}{k_o} \left(\frac{k}{k_o}\right)^4 e^{\left(-2\left(\frac{k}{k_o}\right)^2\right)} \quad (1)$$

k_o is the wave number at the maximum of the spectrum and is dependent on \mathcal{L} :

$$k_o = \frac{8}{3} \sqrt{\frac{2}{\pi}} \frac{1}{\mathcal{L}} \quad (2)$$

Distances are non-dimensionalized by the computational domain length.

The DNS code is employed to compute two-dimensional compressible conservation equations for density, velocity, total energy and mass fraction of the species involved. Those equations can be found in [11]. Complex mixture transport (including Soret effect) and chemistry are used. The numerical method is based on a sixth-order implicit spatial scheme, [14], and a third-order explicit Runge-Kutta time integration with low storage [15]. Boundary conditions are periodic.

The initial dynamic fields are the same in all the simulations. The turbulent Reynolds number is about 22 and the turbulent length scale .08 of the box size. Consistently, the length scales of any initial scalar distribution are fixed as well. They mimic a two-peak distribution whose wavelengths are 6π and 10π . The first peak is chosen as a small wavelength scale compared to the turbulent energy spectrum peak and corresponds to coherent eddies breaking the pockets of scalar. The second one is in the inertial range and initiates micro-mixing. To match the statistic, a β -PDF function based on mean and segregation factor rescales the scalar field. The reader is reported to [16,17] for details of the initial conditions definition used here. Typical pure fumigated fuel temperature is 500 K. Pure air temperature is adapted for different distributions such that the initial box average temperature is kept at 1100 K. Excepted where specified, $\Phi = 1$, $\sigma = .1$.

The chemical schemes are the skeletal ones developed for n-heptane and DME ignition under engine-like conditions [12,13]. The intensive computing demand leads to the use of skeletal schemes; this is another limitation of the presented simulations. N-heptane has a stoichiometry typical of hydrocarbon: .062 while DME, because of oxygen, has a much higher stoichiometry: .1.

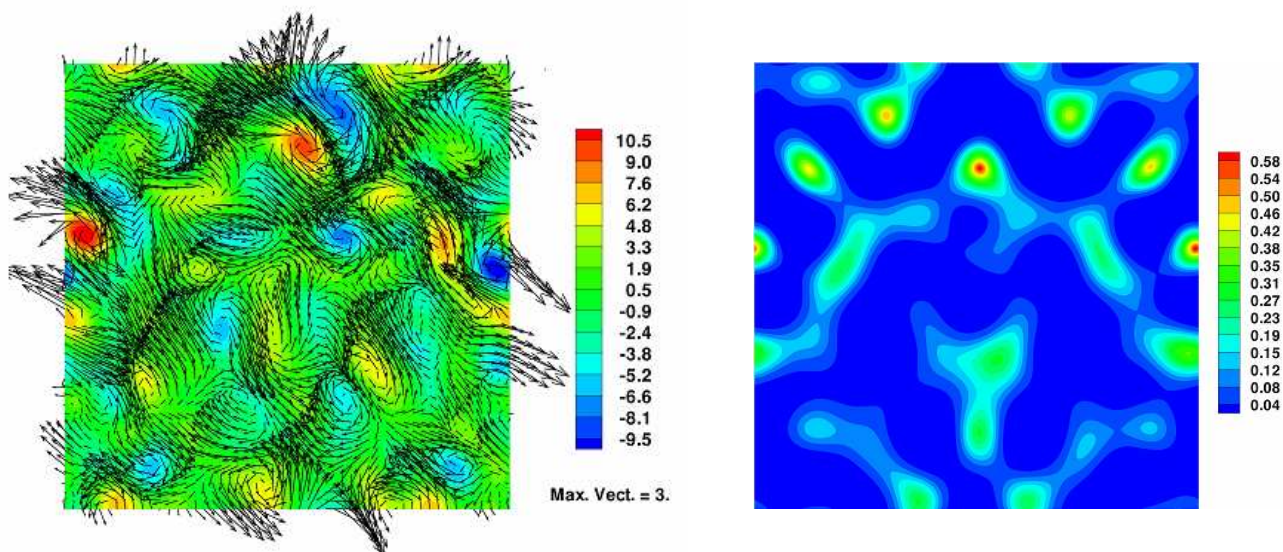


Fig. 1. Initial fields. Left: vorticity (arrows: velocity). Right: mixture fraction. Fields are made non-dimensional by turbulent rms velocity u' and integral length L . N-heptane for low-segregation case (see table imbedded in Fig. 4).

RESULTS

1-D constant-volume ignition tests of the proposed chemical schemes have exhibited underprediction of the ignition delay. The relative difference in ignition of DME with respect to n-heptane at 41 bars and 1100 K is nevertheless preserved. This has been used with profit to separate mixing and chemical time scales, by allowing conducting ignition simulations in non-homogeneous mixture undergoing very high dissipation.

Contours of temperature and ignition-kernel-tracer intermediate species are obtained for both DME and n-heptane in Fig. 2 after five Eddy-Turn-Over Times (E.T.O.T., the characteristic time for an initial eddy to rotate, $= L/u'$). According to these pictures (and within the limit of the chemical description permitted by the mechanism used), OH radicals correlate reasonably well with the hottest spots, pointing out the mixture in ignition. This tracer is more visible in the case of DME than n-heptane, as shown in the figure, because of a slower ignition for n-heptane. When the same advancement in ignition is considered (i.e., mean temperature and no more time is used as the reference variable), OH radicals pockets clearly appear within the ignition kernels as well for n-heptane (not shown here).

According to [12,13], the representative intermediate specie is CH_2O for DME while a direct decomposition into CO can be approximated for n-heptane. *On the basis of these proposed schemes*, area of initiation of both fuels oxidation is provided in Fig. 3 at the same time. The intermediate species are thus good markers of the advancement of the ignition phase [5]. At first, they are signature of the decomposition of the molecule. When ignition is more advanced, they are consumed. Those are the reasons why the intermediate specie maps do not perfectly correlate with the temperature maps, but both draw together a comprehensive pattern of chemical state.

In Fig. 4, the effects of micro-mixing on ignition are illustrated. First, the advantage of high dissipation is highlighted: the time-evolution of the temperature is slow enough to detect all the

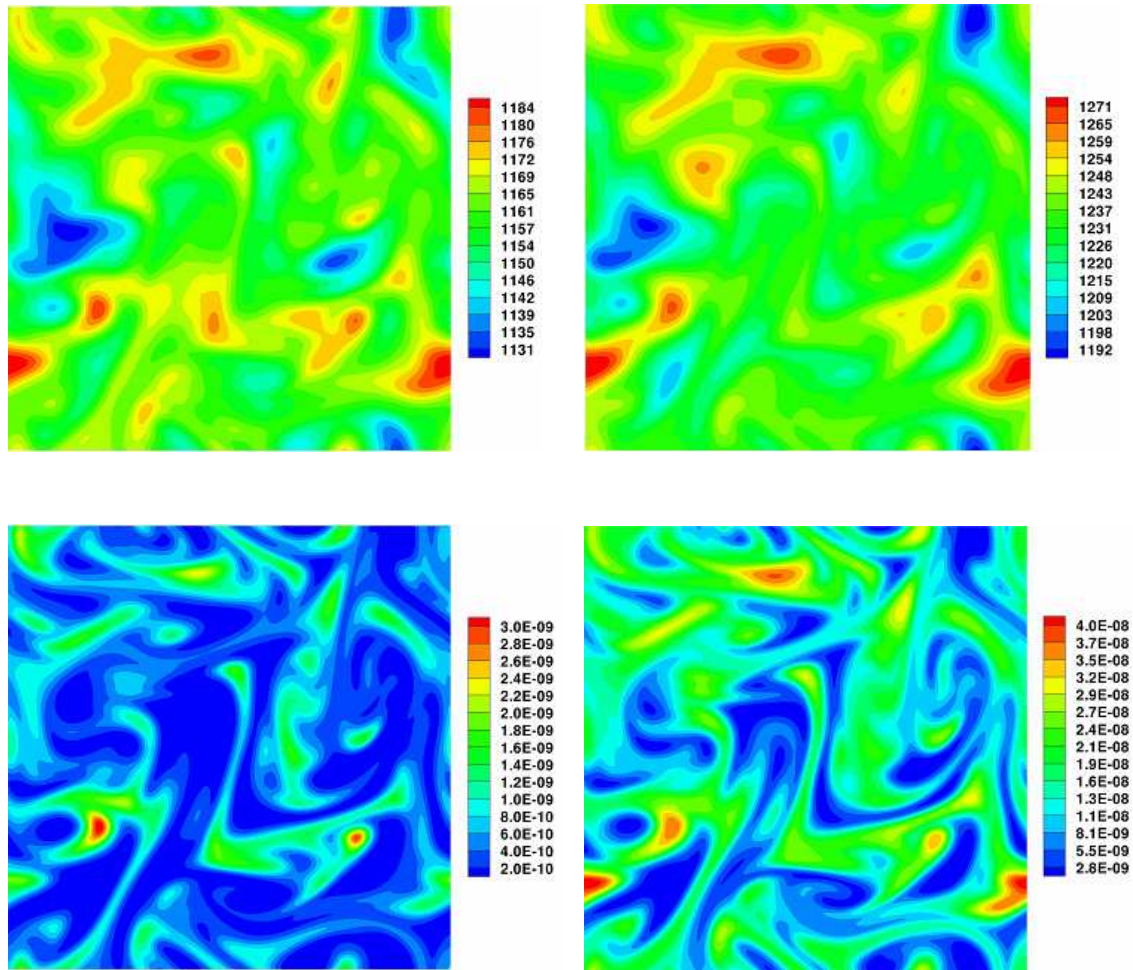


Fig. 2. Temperature (top) and OH radical (bottom) fields for n-heptane (left) and DME (right) after five E.T.O.T.

embedded phenomena. The most important one is the effect of micro-mixing temperature. When the segregation is large enough, ignition is very slow such that the effect of mixing temperature is visible. This is due to the homogenisation of a mixture composed of cold fuel and hot air with different heat capacities. The final frozen mixing temperature is lower than the initial mean temperature in the domain. This cooling delays ignition. It is not visible for lower segregation because: (i) temperature runaway hides it; and (ii) ignition is fast enough to not allow this cooling process such that chemistry is never affected by this temperature decrease. Conditions are here outside of the range of the negative temperature coefficient ignition and there is no benefit for a lower temperature due to mixing.

Another interesting aspect is the comparison between DME and n-heptane ignition for the same initial field (i.e. the mixture is stoichiometric for DME but rich for n-heptane). N-heptane ignition profits for two reasons: (i) n-heptane ignites easier in rich mixture; (ii) in this typical inhomogeneous field, n-heptane concentration iso-lines are pushed towards hot pockets of air. This is due to the difference in stoichiometry between DME (~ 1) and n-heptane (~ 0.062). Thus, when the mixture tends to be rich, inhomogeneities are in favour of ignition of conventional

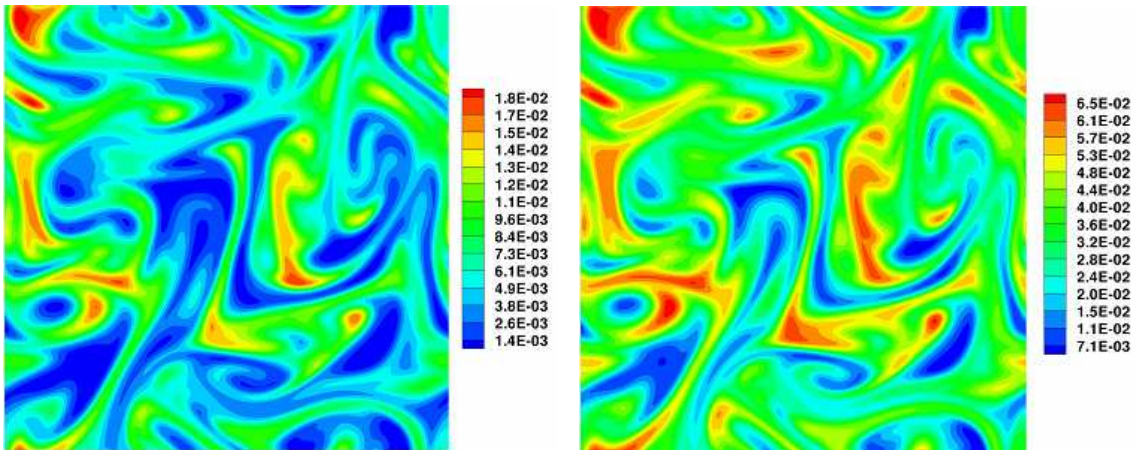


Fig. 3. Mass fraction of CO / n-heptane (left) and CH₂O / DME (right) after five E.T.O.T.

hydrocarbon fuels. This situation happens with the increase of load in diesel engine and is a potential explanation for the observed decreasing discrepancies in ignition time between biodiesel and conventional diesel when more fuel is injected. For biodiesel, a higher cetane number advances the combustion phasing. However, this advance disappears at high load and biodiesel and hydrocarbon both tend to ignite at similar times, according to cylinder data.

CONCLUSION

It has been shown that turbulent mixing in a non-homogeneous field may impact ignition processes of oxygenated fuels. Although DME, like most other alternate fuels, has a relatively large cetane number compared to normal alkane oils, the shift in the stoichiometric value makes it ignite and burn in colder regions. Classical hydrocarbons tend to react on the hot air side. This pattern may explain, at least in part, why the benefit in ignition of biodiesel disappears with the load in a diesel engine, compared to n-alkane oil.

The scalar dissipation rate has the expected qualitative effect. A higher segregation factor delays ignition. It is shown that this effect is particularly sensitive, especially with regard to the existence of a cold-fuel-hot-air mixing temperature which further delays ignition. This subtle effect may be considered in improved combustion models dedicated to HCCI engines. The prediction of the ignition-combustion phase is one of their main issues.

Future work. Methanol is a good candidate for HCCI engines as a renewable fuel. Its tolerance to EGR is an interesting feature. Its high octane number might be controlled through the use of reformat gas. Further work is planned to investigate in depth self-ignition in turbulent non-homogeneous fields of methanol-reformat gas in hot air and under high pressure.

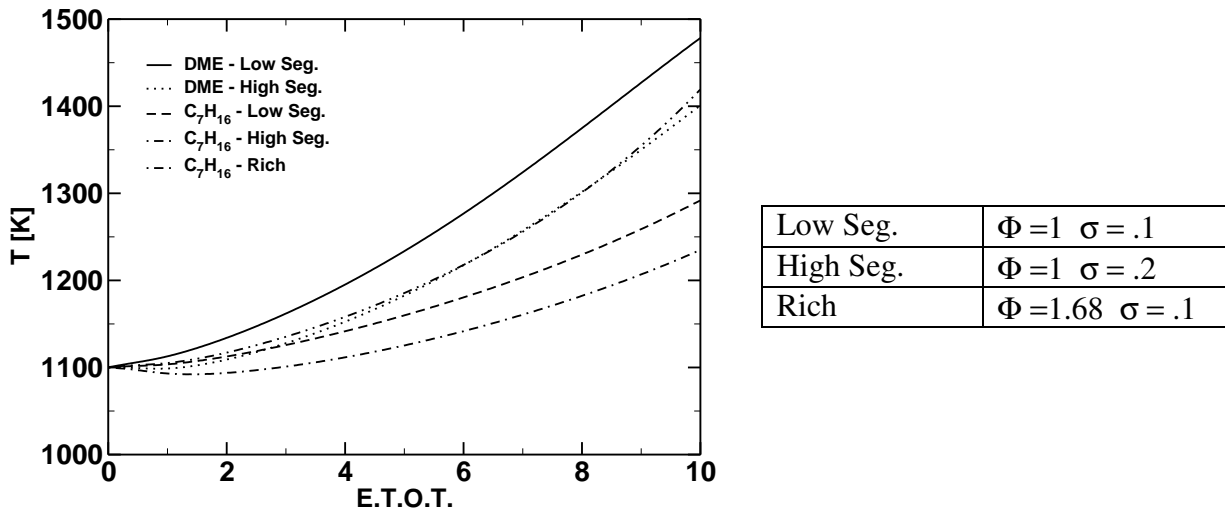


Fig. 4. Mean temperature *versus* time for different initial fields and fuels.

REFERENCES

1. Chen, J., Hawkes, E., Sankaran, R., Mason, S., and Im, H., *Combust. Flame*, In Press.
2. Hawkes, E., Sankaran, R., Pébay, R., and Chen, J., *Combust. Flame*, In Press.
3. Sankaran, R., Im, H., Hawkes, E., and Chen, J. (2004). *Proc. Comb. Inst.*
4. Echekki, T., and Chen, J., *Combust. Flame* 169:191 (2003).
5. Wang, Y., and Rutland, C. (2004). *Proc. Comb. Inst.*
6. Wang, Y., and Rutland, C. (2005). *J.o.P.: Conference Series*.
7. Viggiano A., and Magi, V., *Combust. Flame* 432:443 (2004).
8. Kong, S.-C., and Reitz, R. (2002). *Proc. Comb. Inst.*
9. Kong, S.-C., and Reitz, R., *Combust. Theory Modelling* 417:433 (2003).
10. Guichard, L., Réveillon, J., and Hauguel, R., *Flow Turb. Comb.* 133:167 (2004).
11. Kuo K. (1986). *Principles of combustion*.
12. Nordin, N., and Golovitchev, V. (1997). *The 7th International KIVA Users Meetings*, SAE Congress.
13. Golovitchev, V., Nordin, N., and Chomiak, J. (1997). *SAE Int. Spring Fuels & Lubricants Meeting & Exposition*.
14. Lele, S., *J. Comput. Phys.* 16:42 (1992).
15. Wray, A. (1990). *Tech. Rep.*, Center for Turbulence Research, Stanford University.
16. Réveillon, J. (1999). *Ph.-D. thesis*.
17. Vervisch-Guichard, L. (1999). *Ph.-D. thesis*.