NUMERICAL INVESTIGATION OF IGNITION DELAY TIMES IN A PSR OF GASOLINE FUEL

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Abstract
This paper reports on preliminary results of a study conducted by simulating the ignition of a flammable mixture of gasoline and air, in a perfectly stirred reactor (PSR). Several ignition conditions have been analyzed by varying the initial temperature, the pressure and the equivalence ratio and temperature of the feeding mixture. The fuel has been described with a surrogate composed by a mixture of n-heptane, toluene and iso-octane. The detailed chemical mechanisms proposed by the CRECK group of Politecnico di Milano, the POLIMI-TOT-NOX-1407, consisting of 484 species and 19341 reactions has been adopted to achieve a high fidelity in the reproduction of the ignition delay time.
The effect of mixture composition, pressure, initial temperature and residence time is illustrated. It is shown that significant deviations from the ignition delay time (IDT) measured in batch reactor arise. The dependency shown upon the parameters space can be of great help in explaining the ignition behavior in real engines, which is often difficult to interpret.

Introduction
Ignition Delay Time (IDT) is a fundamental property of a flammable mixture that has a strong influence on the performances of transportation engines [1]. It is extensively adopted also to test the performances of chemical mechanisms aimed at miming the behavior of real fuels [2]. Because ignition always starts at temperatures lower than the final temperature reached after the thermochemical conversion, a proper representation of the low temperature chemistry is required to achieve correct predictions; a very difficult task especially starting from ambient conditions [3].
IDT, whose exact definition is not univocal, can be determined by measuring the spontaneous evolution of the mixture in batch conditions, experimentally realized in batch reactors or, for higher initial temperatures, in shock tubes. The same conditions are numerically realized by the constant pressure batch reactor model, fixing the initial conditions of the mixture. However, in real conditions, almost never this is the effective evolution experimented by the mixture: in combustors, where a regime of steady ignited conditions is eventually desired, the ignition is an unsteady process occurring in a flowing reactor at constant pressure, during the continuos mixing with a fresh mixture; in spark ignited Internal Combustion Engines, a flame develops at

every cycle within a highly recirculating flow at variable pressure and temperature, thus continuously varying the conditions of subsequent ignition of the propagating flame. Therefore, while IDT in batch conditions are of paramount importance to establish fundamental properties of the mixture chemical behavior, the connection with ignition conditions in practical devices is weaker.

Ignition conditions closer to those just described for combustors can be reproduced in an unsteady Perfectly Stirred Reactor (PSR). This reactor, extremely simple yet, include the effect of a flowing stream and therefore the ignition phenomenon can be studied in a wider range of conditions that include, further to initial mixture equivalence ratio, pressure and temperature, also the composition and temperature of the feeding mixture, and the residence time in the reactor. The interplay of this parameters leads to much complex interactions driving the chemical evolution of the reactive mixture that, even if a 0-Dimensional description of the system is adopted, have resemblance with the inner chemical portion of a flame structure propagating in a not homogeneous field.

This paper reports on preliminary results of this study. Several ignition conditions of a gasoline-air mixture in a PSR have been simulated by varying the initial temperature and the equivalence ratio of the feeding mixture, the feeding temperature and mixture composition, and the pressure. The effect of mixture composition, pressure, initial temperature and residence time is illustrated. It is shown that significant deviations from the IDT measured in batch reactor arise.

Mathematical Model

The governing ordinary differential equations of the adiabatic, constant pressure PSR fed by a mixture of N_S species with mass fraction Y_i, molecular weight W_i and temperature T, can be given as [4]:

$$\frac{dY_i}{dt} = \frac{Y_{i,f} - Y_i}{\tau} + \frac{W_i r_i}{\rho V} \quad , \quad i = 1, \dots, N_S \tag{1}$$

$$\frac{dT}{dt} = \sum_{i=1}^{N_S} \frac{Y_{i,f}(h_{i,f} - h_i)}{\tau \, c_P} - \sum_{i=1}^{N_S} \frac{W_i r_i h_i}{\rho V c_P} \tag{2}$$

where h_i are the enthalpies of species i, r_i the their reaction rate. The subscript f indicates the feeding (inlet) conditions and $\tau = \rho V / \dot{m}_f$ is the nominal residence time and related to the reactor volume (V) and the mass flow rate ($\dot{m}_f$). c_P is the constant pressure specific heat coefficient of the mixture.

Mixtures formed by air and gasoline are considered. Air is supposed to have 76.7 % mass of nitrogen and 23.3 % mass oxygen. The fuel has been described with a surrogate composed by a mixture of n-heptane, toluene and iso-octane ($0.630 \, iC_8H_{18} + 0.200 \, C_7H_8 + 0.170 \, nC_7H_{16}$) [5]. The detailed chemical mechanisms proposed by the CRECK group of Politecnico di Milano [], the POLIMI-TOT-NOX-1407, composed by 484 species and 19341 reactions has been

adopted to achieve a high fidelity in the reproduction of the ignition delay time.
The IDTs in the PSR (PSR-IDT) at different working conditions have been obtained by computing the time instant of the maximum in the signal of temperature rise velocity. However, every simulation has been successively verified to filter out cases with failed ignitions.

Results

PSR-IDTs have been evaluated at different residence times assuming that only air is initially present in the reactor while the reactor is fed with the flammable mixture. With respect to an auto-ignition process in a batch reactor, the ignition in this configuration differs substantially. The most influencing factors are expected to be the time required to supply the inflammable mixture and the heat loss determined by the outflow of the expanding mixture.

Typical ignition curves versus time are represented in Fig. 1 for $P = 48$ atm, $T_i = 1200$ K, $T_0 = 1000$ K, $\varphi = 1$, and different values of τ. To make comparable the different cases, the time has been non-dimensionalized with the respective residence time. It is recognized that the ignition process is quite different changing the residence time. Two different stages are recognized, a fast (that occurs in a time shorter than the residence time) and a delayed stage.
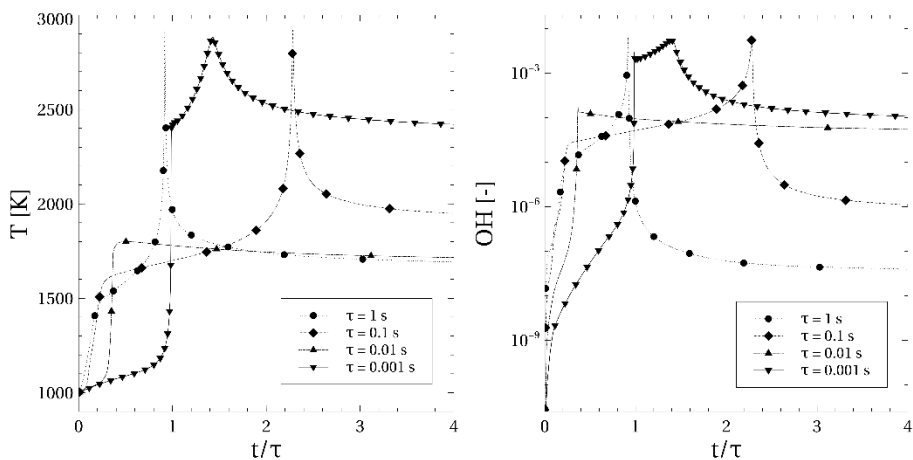

Figure 1. Time evolution of the temperature (left) and OH mass fraction (right) versus non-dimensional time.

A complete picture of the conditions for which the ignition of the mixtures is possible is given in Fig. 2. Several trends can be recognized, mostly confirming expectation. As expected, an increase of the temperatures, both T_0 and T_{in}, favors ignition. Residence time and inlet temperature play a major role: ignition becomes very difficult, and allowed only at the highest inlet temperatures, when a very short residence time is considered. Higher pressure always enlarges the region of ignition. The mixture composition has a very little effect at the lowest residence times, while

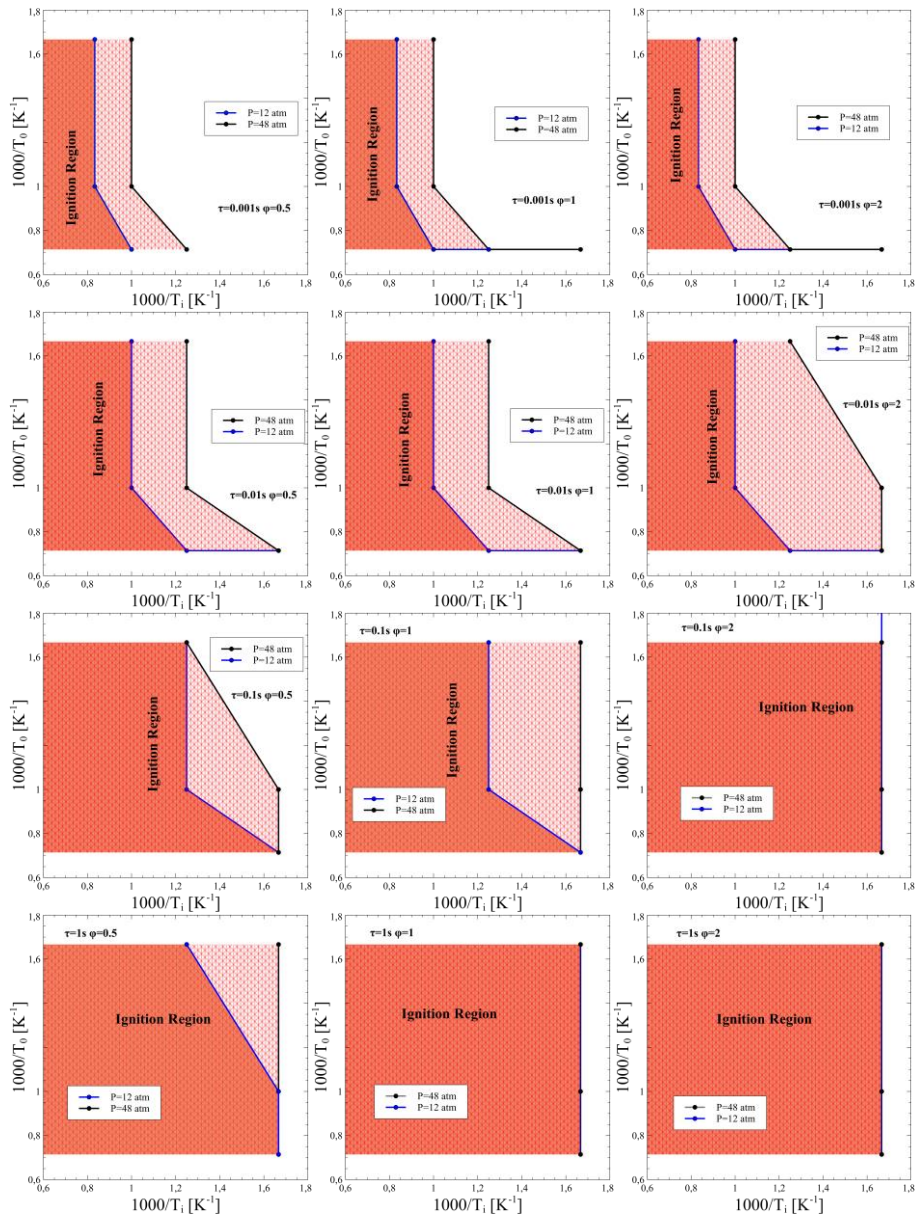its effect is significant especially at intermediate residence times.

Figure 2. Ignition maps in the temperatures plane (1000/T_{in}, 1000/T_0) at pressures of 12 and 48 atm. From top to bottom is increasing residence time. From left to right is increasing equivalence ratio.

In these cases, the ignition is favored by rich mixtures. This is easily explained in coupling with the initial, pure air, content of the reactor: a flammable mixture more rapidly forms in the reactor during the first instants, and the heat released helps the stabilization of ignited regime conditions.
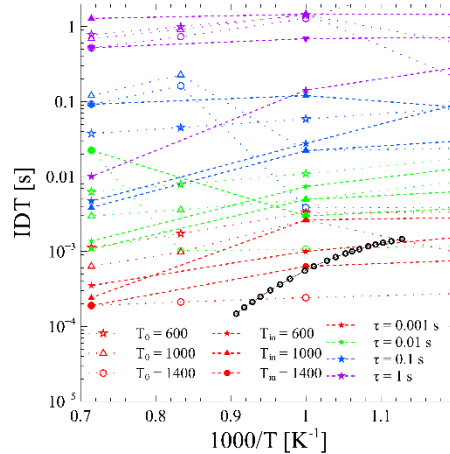

Figure 3. IDT for a stoichiometric mixture from experiments in batch reactors (black circles, adapted from [], high pressure conditions) and IDT from present computations in PSR, $P = 48$ atm (colors are for different residence times, empty symbols for constant T_{in}, filled symbols for constant T_0).

Figure 3 reports the PSR-IDT computed at $P = 48$ atm for a stoichiometric mixture using different residence time, and different initial and feeding temperatures. For comparison, classically defined IDT in a batch reactor at the same stoichiometric and pressure conditions are also reported. Several interesting observations can be made. The PSR-IDT initially filled with air mainly depends on the residence time and is very roughly proportional to this parameter: about an order of magnitude can be expected by changing the temperatures but it is difficult to observe the ignition of the mixture in a time much shorter than $1/10t$ even at the highest temperatures. Following these indications, ignition delay times in real devices could greatly differ from the ideal IDT. The effect of changing T_{in} at constant T_0 (empty symbols in Fig. 3) is very weak. Instead, significant variations are found by changing the initial temperature in the reactor. This can be interpreted by observing that, due to the immediate mixing of the feeding mixture with the mixture in the reactor at the beginning of the phenomenon, the temperature of the latter mixture predominates in the first ignition stage. Instead, successful ignition is mostly dependent on the feeding temperature, because of the role of the feeding mixture energy content in sustaining the reaction progress.

Conclusions

The paper illustrates the first preliminary results obtained from the study of the ignition process of a gasoline in a constant pressure PSR. Several important indications are deduced from this kind of analysis, that can extend the importance of the study of IDT in batch reactors. For instance, it has been shown that the PSR-IDT is roughly proportional to the residence time, thus implicating that low temperature chemistry can be sustained in a time interval much longer than that observed in batch reactors. Furthermore, the chemical evolution in this kind of reactor involves a much larger spectrum of mixtures composition, due to the continuos feeding of the reactants. It makes possible the observation, in a zero-dimensional reactor, of a large variety of reaction conditions, including those involving the combination of molecules formed during initial dissociations with molecules formed during the last stages of products formation.

Acknowledgements

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Errata corrige

Because of a last minute mistake, the images reported for Fig. 1 in the submitted paper were taken from a wrong directory, where not converged solutions where saved. The system of ODE integrated is very stiff and a careful check of each solution was needed to purge not converged results, a not trivial task because of the large number of solution processed. The correct Fig. 1is here below reported.
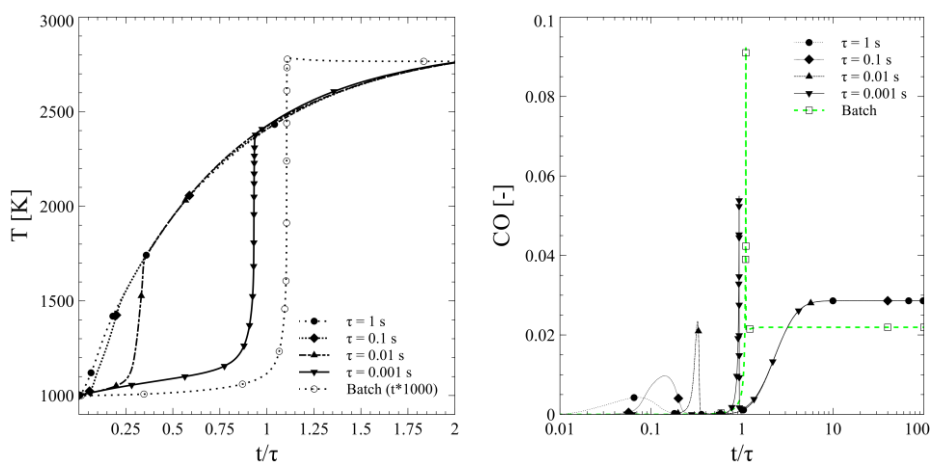

Figure 1. Time evolution of the temperature (left) and CO mass fraction (right) versus non-dimensional time.