



## Propane oxidation in a Jet Stirred Flow Reactor. The effect of H<sub>2</sub>O as diluent species

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### ABSTRACT

Advanced combustion technologies, such as MILD, LTC (Low Temperature Combustion) reduce emission of pollutants by controlling system working temperatures to values not critical to promote the formation of several classes of pollutants. To access this temperature range, a significant dilution of reactants is required. At the same time, reactants have to be preheated to sustain the oxidation process. Such conditions are achieved by a strong recirculation of exhaust gases. Such a strategy implies that high contents of CO<sub>2</sub> and H<sub>2</sub>O interact with reactants oxidation chemistry. In order to characterize this aspect of the combustion processes under diluted conditions, experimental tests were carried out for propane/oxygen/nitrogen mixtures in presence of variable amounts of H<sub>2</sub>O in a quartz Jet Stirred Flow Reactor (JSFR). Experiments were carried out at atmospheric pressure, over the temperature range 720–1100 K, from fuel lean to rich conditions and at a residence time of 0.5 s. Temperature and species concentration measurements suggest that the oxidation of propane is significantly altered by H<sub>2</sub>O in dependence of mixture inlet temperatures and equivalence ratios.

Numerical analyses were performed to explore the interaction of H<sub>2</sub>O with the oxidation chemistry of propane. Results suggested that such a species alters the main radical branching mechanisms, i.e. in termolecular reactions as a third body species with high collisional efficiency or directly participating in bimolecular reactions.

### 1. Introduction

Innovative combustion technologies for power generation in the industrial, domestic, and transport sectors are required to meet the needs of high energetic efficiency and low pollutants emissions, and they have to be flexible with respect to the fuel nature.

Diluted combustion strategies (MILD, LTC, etc.) are receiving increased attention as means to reach such targets, as the resulting peak flame temperatures are low to promote the NO<sub>x</sub> and soot formation. To access this temperature range, significant dilution as well as preheating of the reactant mixtures is required. In practical systems, dilution and preheating are usually achieved through internal or external exhaust gas recirculation [1,2].

Therefore, these combustion processes occur in presence of great amounts of carbon dioxide and water. Such species may have thermal and chemical effects [3–5].

Lubrano Lavadera et al. [6] provided a summary of the experimental and numerical studies to date, which have investigated the

effects of CO<sub>2</sub> on combustion properties. They studied the effects of significant additions of CO<sub>2</sub> on propane oxidation in a JSFR at atmospheric pressure. They found that propane oxidation is significantly altered by CO<sub>2</sub> in dependence of mixture inlet temperatures and equivalence ratios.

Recently, mixtures of fuels with H<sub>2</sub>O have received attention. In the scientific literature, several works have been reported on the study of laminar flame speeds and extinction strain rates [7–9] for fuel mixtures partially diluted in H<sub>2</sub>O because of the increasing interest in Low Calorific Value (LCV) fuels. The common statement is that the H<sub>2</sub>O significantly reduces the burning velocities and the extinction strain rates of these mixtures. Indeed, H<sub>2</sub>O decreases the flame temperature, thus the fuel oxidation reaction rate. For systems working at high temperatures, it has also been pointed out that H<sub>2</sub>O is not inert but directly participates in chemical reactions. Water addition was found to dramatically reduce H and O mole fractions while increasing OH ones, mainly due to H<sub>2</sub>O + O = 2OH [9].

Anderlhor et al. [10] numerically investigated the thermal and

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kinetic impact of the residual species CO, CO<sub>2</sub> and H<sub>2</sub>O on the oxidation chemistry of n-heptane/iso-octane/toluene blends at high dilution ratio (97%) from low to medium temperatures (650–1100 K) at atmospheric pressure. These operative conditions are relevant for the post-oxidation zone in IC engines. They found that the H<sub>2</sub>O thermal effects inhibited the oxidation process instead of the kinetic one mainly because of the third-body reactions. They showed the importance of H<sub>2</sub>O<sub>2</sub> dissociation at low and intermediate temperatures. The authors suggested revising the efficiencies of the potential collision partners.

Abián et al. [11] investigated the oxidation of CO in a quartz flow reactor that operated at atmospheric pressure over the temperature range of 700–1800 K from fuel-rich to fuel-lean conditions in the presence of various amounts of CO<sub>2</sub> and H<sub>2</sub>O, representing different exhaust-gas recirculation conditions. In contrast with other works, the authors found that H<sub>2</sub>O enhances the CO conversion. They optimized the H<sub>2</sub>O third-body efficiency in reaction  $H + O_2 + M = HO_2 + M$  in the detailed kinetic mechanism that they used and multiplied its efficiency for a correction factor.

Sabia et al. [12] studied the effects of significant additions of CO<sub>2</sub> and H<sub>2</sub>O on propane autoignition delay times for temperatures ranging from 850 K to 1250 K and atmospheric pressure. Significant changes of autoignition delay times were observed for the mixtures compared with N<sub>2</sub> measurements, which were not captured by available kinetic models. The disagreement between experiments and model predictions was found even more evident when studying, in the same conditions, the ignition of a model gas surrogating the gaseous fraction of biomass pyrolysis products [13].

In all the cited papers, the authors recommended further investigation of the effect of higher concentrations of H<sub>2</sub>O in the reactive mixture, as models need additional validation in this parameter space. Several reasons have been proposed to explain these discrepancies, including the sensitivity of rate coefficients at low-temperature/diluted conditions [7].

There are two major distinctions about the low temperature reactions when compared with the higher temperature classifications. The degradation of the hydrocarbons (involving both abstraction and addition processes) tends to follow a sequential breakdown of the carbon backbone (such as  $C_4 \rightarrow C_3 \rightarrow C_2 \rightarrow C_1$ ) rather than the easy fragmentation into smaller carbon-containing units that may occur at higher temperatures ( $C_4 \rightarrow 2C_2$ , for example). Thus, simplifications of the kind that are employed at higher temperatures, as a result of common structures within certain classes of reactions, are not so readily applicable. Also, the selectivity of reactions of different propagating free radicals (especially OH, HO<sub>2</sub>, RO<sub>2</sub> or RO) is so much more marked, and also the reactivity at particular C–H bonds have an increased importance at low temperatures because the relative magnitudes of rate constants for individual reactions are so much dependent on the activation energies in the Arrhenius expression at lower temperatures [14]. Kinetic models require reaction rate, thermochemical, and transport data for the rapidly growing number of species and reactions present. Unfortunately, only a relatively small proportion of reactions now included in comprehensive kinetic schemes actually have been studied directly by experiments. Theoretical methods for calculating reaction pathways and rates of reaction have been developed, many of which now require supercomputer resources to solve the complex quantum mechanical systems involved. Thus, there is considerable recourse to estimation techniques for reaction rates and thermochemical quantities required by models [15].

Therefore, fundamental study is necessary to understand the mechanisms of non-conventional combustion phenomena. The understanding of such phenomena must rely on validated detailed reaction models established for non-conventional conditions than those conventionally addressed. To assist the development and validation of more reliable chemistry models, new experiments are required, spanning as many different types of practical systems and as wide a range of conditions as possible.

Given this background, the objectives of the current work were to investigate the effect of H<sub>2</sub>O dilution on the concentration profiles of chemical species and how it depends on process parameters, including data obtained in a JSFR, at conditions relevant to diluted combustion. The experiments were carried out for lean, stoichiometric, and rich mixtures, diluted with N<sub>2</sub> and two mixtures of N<sub>2</sub> and H<sub>2</sub>O, at atmospheric pressure. The study bridges the region between low and intermediate temperature conditions of practical interest to diluted combustion applications. Propane was chosen as the reference fuel because its chemical kinetics is fundamentally important for all combustion processes of hydrocarbons, is well known, and is sufficiently simple. Moreover, propane reflects the thermochemical and combustion properties of larger hydrocarbons.

Obtaining such measurements was the primary objective of the present study. They provide validation targets for detailed kinetic mechanisms development.

In addition, the performance of updated kinetic models in predicting the experimental data was tested. The experiments do not only provide data for models validation, but also contain information in itself. Therefore, numerical analyses were performed to gain an understanding of the contribution of these non-conventional conditions on the combustion chemical kinetics. Finally, possible sources of disagreement between the model predictions and experimental data were outlined.

## 2. Experimental and numerical tools

The oxidation of propane was studied in a JSFR; it approaches the behavior of an ideal Perfectly Stirred Reactor (PSR). The JSFR is an important experimental tool in kinetic studies because it allows for an accurate monitoring of the extent of reaction, focusing only on chemical kinetics phenomena. The apparatus consists basically of a gas feeding system, a JSFR reactor and a chemical gas analysis system.

The reactor [16] consists of a sphere of 113 cm<sup>3</sup>. It is made in quartz to prevent catalytic reactions. The main flow is composed by oxygen and diluent. It passes through a quartz tube located within two cylindrical electrically heated ceramic fiber ovens. The main flow residence time within the quartz tube and the installed electric power are designed to reach pre-heating temperatures up to 1250 K. It subsequently mixes with the secondary flow, composed by fuel and diluent, in a premixing chamber. Then the pre-mixed mixture enters the reactor through four nozzles of 1 mm diameter located at its center. The well mixing of the reactor was verified in the past by means of pulse tracer experiments following a procedure described by Levenspiel [17]. The results suggested that the reactor behaves as a PSR for residence times lower than 0.6 s. The residence time used in the present experiments was thus fixed to 0.5 s. Under these conditions, the mean residence time differs from the ideal PSR residence time of about 3%. The residence time of the fuel mixture in the injector is more than 100 times lower than the mean residence time in the reactor. Thus, oxidation of the fuel inside the injector is prevented. The products of combustion were exhausted through a 3 mm diameter tube located at the bottom of the reactor. The reactor is located within other two electrical fiber ovens to minimize heat loss to the surroundings. A recirculation air system provides a homogeneous temperature distribution in the oven. The homogeneity of the reactor wall temperature is monitored with movable thermocouples. The temperatures of the reactor wall and of the gases upstream are measured by type N thermocouples and regulated by PID controllers.

The flow rates of gases from cylinders are measured and regulated by digital thermal mass flow controllers supplied by BronkHorst High-Tech with a high accuracy ( $\pm 0.5\%$ ). The controllers are connected to a PC and managed by sub-routines developed in Labview. The pressure is kept constant at 1.1 atm in the apparatus by means of a needle valve on the exhaust gas line.

Gases were provided with high purities: 99.999% for nitrogen,

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