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# COMPARISON OF KINETIC MECHANISM PREDICTIONS OF IGNITION DELAY TIME AT HIGH PRESSURE FOR PARTIALLY-CRACKED AMMONIA

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## INTRODUCTION

Today, the urge to replace fossil fuel is more important than ever before. Ammonia is a good candidate as not only a hydrogen carrier but also as a carbon free fuel itself since it is already largely synthesised, easily transportable and storable. However, ammonia can be blended with Hydrogen (H<sub>2</sub>) or partially cracked (NH<sub>3</sub> 3/2 H<sub>2</sub>+ 1/2 N<sub>2</sub>) to enhance ammonia combustion's properties but unfortunately favouring the knock phenomena. To predict this phenomena, Ignition Delay Times (IDTs) have to be well simulated at high pressure (40-70 bars) and medium temperature (950 to 1050 K). From literature, IDTs are available at this initial pressure range between 40 and 70 bars but not with 2.5 to 5% of cracked ammonia. During this study, a Rapid Compression Machine was used to expand this database with this pressure range and medium temperature for ammonia blended with hydrogen in order to determine which kinetics mechanism can agree accurately.

## SETUPS AND METHODOLOGY

Experiments were performed on a Rapid Compression Machine (RCM), which compresses a gas in less than 33 ms. This RCM is pneumatically driven and equipped with a stroke of 300 mm while the bore is 50 mm diameter. Dead volumes can also be adapted by means of some additional spacers to obtain the desired compression ratio of 11.75. The piston is braked, close to the top dead centre, in an oil chamber. The RCM is equipped with a Kistler 6054BRU59-3-1 pressure sensor with a 0-300 bars range and a linearity of 0.2%. To provide consistent experimental data and perform simulations, a first experimental campaign was done with non-reactive blends, i.e., by replacing oxygen (O<sub>2</sub>) by nitrogen (N<sub>2</sub>) to unblock the oxidation reaction but to keep an equivalent global heat capacity and thus measuring thermal losses and pressure evolution inside the combustion since non-reactive experiments are strictly identical in terms of temperature, pressure and composition to reactive experiments. Then the second experimental campaign was performed with reactive blends i.e. with ammonia (NH<sub>3</sub>), hydrogen (H<sub>2</sub>) and nitrogen (N<sub>2</sub>) at various percentage, oxygen (O<sub>2</sub>) and argon (Ar), to replace nitrogen content in the air, for the reactive blend. Ar is used in this study to easily reach high temperature since its heat capacity is twice lower than nitrogen's. As soon as the tank is filled as desired with the

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various gases, vacuum is made inside the combustion chamber. Then, the piston is set to its initial position before the combustion chamber is fuelled in with mixed gases. Once the initial pressure is reached, the intake valve is closed and the piston is released to compress gases. The oxidation occurs in the second campaign tests which produce a brutal pressure rising. From this, an IDT can be measured between the end of the compression and the maximum pressure gradient.

Simulations are performed by using ChemKin Pro ANSYS software. Reactive initial conditions, pressure evolutions obtained with non reactive compositions and the kinetic mechanism tested are implemented inside the Closed Homogeneous Batch Reactor software's module to obtain the simulated IDT. The closest this simulated IDT is to experiments and the better the mechanism is. One way to rank the different kinetic mechanisms is to use Kawka's method, but, this method can only be used for non-null Standard Deviation. However, simulations or experiments can lead to no ignition, in this case, IDT value is arbitrary set to 1 second, Standard Deviation is therefore null. A new quantification method was then developed based on Kawka's one. The aim is to compute the relative error between experimental and simulated IDTs for each set and then to average it for each temperature at a given pressure and equivalence ratio ( $E\Phi, P, T$ ). Then, average the previous result for each pressure at a given equivalence ratio ( $E\Phi, P$ ). Finally, it is possible to average all  $E\Phi, P$  to obtain a relative error for each equivalence ratio ( $E\Phi$ ).

## RESULTS AND CONCLUSION

Almost all mechanisms predictions are better for cracked ammonia than pure ammonia. However, reaching 5 % of cracked ammonia does not necessarily mean that mechanism do better predictions. For some of them, predictions are better with 2.5% cracked than 5% cracked. However, when partially cracked ammonia is added, many mechanisms predict IDTs with less than 100% relative error.