Comparison of Experimental and Numerical Results of the Autoignition of n-Heptane Sprays under Machine Conditions

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Abstract
Modern aircraft turbines, which inject liquid hydrocarbon fuels into compressed air at high temperatures, aim for a high compression ratio on the order of 40 to 45 to achieve high process efficiency. This means there is only a limited residence time of the fuel in the combustion chamber before autoignition. The residence time however is important in terms of vaporizing and turbulent mixing of the fuel with air. A well stirred mixture with a lean overall equivalence ratio (near the adiabatic flammability limit) will reduce the combustion temperature and in turn reduce the production of nitric oxides (NO, N₂O and NO₂) through the Zel’dovich mechanism. This report details some of the results obtained under the ESA MAP project CPS (Combustion Properties of Partially Premixed Spray Systems), where (amongst other topics) n-heptane sprays are observed under machine conditions and these experimental results are compared to numerical results obtained with the ZARM closed vessel code for single droplet ignition.

1. Introduction
This paper represents the first attempt by the combustion group at the ZARM to use the newly operational experimental facility (Hot-Wind-Tunnel, HWK) to compare ground based spray autoignition experiments with numerical results of the closed vessel code39. The results from the closed vessel code can of course only be compared to a uniform mono-disperse spray, however the comparison of the real spray experiments with the results from the numerical simulation still show interesting results, which can help in the development of a more complex model to fully describe spray autoignition.
This in turn is very useful for the development of combustion machines which can reduce the production of nitric oxides if a well stirred lean mixture is provided.

2. Experiment
The experiments were conducted at the Bremen Hot-Wind-Tunnel (HWK), which functions as a Ludwieg tube (Fig. 1), with the test section (336mm diameter and 3000mm length) being in the high pressure section of the wind tunnel. This allows the creation of steady state high pressure, high temperature flows (up to 50bar, 1000K and 100 m/s) for up to 100ms.
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The large test section of the HWK allows the creation of large sprays without the danger of wall impingement. To completely eliminate the danger of fuel igniting on contact with the walls the test section (walls and air) is always kept at temperatures below 373 K, prior to the experiment.
Data acquisition is done at a rate of 10 kHz for pressure and temperature data and the detection of the ignition is done via photodiodes, which also have a sample rate of 10kHz. The injection of the fuel is observed by an Ultima 512 high speed CMOS camera at a frame rate of 8000 fps. In addition to this a CCD Camera (200 fps) was used to observe the injection and ignition of the spray along the axis of the wind tunnel.
The fuel is injected in a jet-in-cross-flow configuration with the help of a pneumatic injection system that allows injection pressures of up to 200 bar, a variation of the fuel temperature (in a range of 273 K to 373 K) and variation of the fuel volume (up to about 5ml, per experiment).

Fig. 1 Operation principle of a Ludwieg tube
The parameters for the experiments in this paper were as follows:

- Pressure of 5 bar
- Temperature range from 650 K to 800 K
- Flow speed about 26 m/s
- Fuel, n - Heptane (0.5 ml)
- Fuel Temp. range from 280 K to 310 K
- Injection pressure 25 bar (absolute)
- Nozzle 0.5mm

3. Spray Classification

With the current configuration of the HWK it is unfortunately not possible to measure the droplet sizes and distributions. This is due to many factors among others the extreme conditions and changes in refraction index in the wind tunnel during the experiments, which make it extremely challenging for any optical measuring technique to acquire a clear signal.

Lacking such technology it is was nonetheless important to have some notion of the parameters of the spray that will be present during the experiments. In order to do this a simple empirical model (ELKOTB 1982) is used to describe the spray:

\[
\text{SMD} = 3.08 \nu^0.385 (\sigma \rho_L)^{0.737} \rho_G^{0.06} \Delta P_L^{-0.54}
\]

Where, SMD is the Sauter Mean Diameter, \( \nu \) is kinematic viscosity (m²/s), \( \sigma \) surface tension (kg/s²), \( \rho \) density (kg/m³) and \( \Delta P \) differential pressure (Pa), the subscripts L and G denoting liquid and gas respectively.

With this model and for the above mentioned conditions a SMD of about 43\( \mu \)m can be obtained.

In addition to the above model the spray break-up mechanism was also classified in order to have a more complete understanding of the problem. This was done using the empirical model developed by Czerwonatis et al. (2000)\(^3\), which extends the classical Ohnesorge – Reynolds number diagram to higher pressures than ambient:

\[
Z^* = \text{Oh} \cdot \sqrt{\frac{We_G}{\eta_L \eta_G}} \cdot \frac{\eta_L}{\sigma} \cdot \frac{\rho_G}{\rho_L} \cdot \frac{\eta_L}{\eta_G}
\]

Where Oh is the Ohnesorge number, We is the Webber number and \( \eta \) is the dynamic viscosity (kg/m s) and again the subscripts L and G for liquid and gas.

With this information plotted against Reynolds number one can classify the spray break-up mechanism either as Rayleigh, wind induced or spray and as can be seen from Fig. 3, the spray break-up in this experiment is wind induced, meaning the above calculated SMD probably represents an upper limit rather than the norm.

In addition to the classification of the spray it was also necessary to have an idea of the overall air/fuel ratio. In order to estimate this a simple geometrical relationship has been used (Fig. 4).

The fuel is injected for a certain amount of time and the spray adopts the flow speed and a roughly circular cylinder is formed which is occupied by fuel and air. The diameter of this fuel-air occupied volume can be directly measured with the imagery from the high-speed cameras.

If one now assumes that only the fuel and air within this cylinder interact and since the injected fuel mass as well as the conditions of the air in the wind tunnel are known it is possible to estimate the overall equivalence ratio.

For the experiment conditions mentioned in this paper this gives a value of \( \varphi = 0.45 \) or \( \lambda = 2.2 \).

4. Numerical

The numerical model used for this study was introduced by O. Moriue et. al.\(^1\). In the Closed Vessel Model a single (cold) fuel droplet is placed at the centre of a constant volume, the vessel (filled with a quiescent
hot ambient gas), is closed against mass, species and energy transfer. The model is fully transient. In both of the phases, liquid and gas phase, mass, species and energy conservation are considered. Moment conservation is neglected as well as thermal diffusion, radiant heat flux, the kinetic energy term, viscosity and body force. The governing equations are solved in spherical coordinates in which spherical symmetry is assumed:

\[
\frac{\partial}{\partial t} \rho + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho v) = 0
\]

\[
\frac{\partial}{\partial t} (\rho Y_i) + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho Y_i (v + V_i)) = w_i
\]

\[
\frac{\partial}{\partial t} (\rho h) - \frac{\partial p}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \sum_i \rho Y_i h_i (v + V_i) \right) = -\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 q_T \right)
\]

Where \( t \) is the time, \( r \) the radial coordinate, \( \rho \) density, \( v \) mass-averaged velocity, \( Y_i \) mass fraction, \( V_i \) diffusive velocity, \( w_i \) mass production by reaction per unit volume and time, \( h \) specific enthalpy, \( p \) pressure and \( q_T \) is the conductive heat flux. Subscript \( i \) denotes species \( i \).

In the liquid phase the only species is n-heptane. Pressure is assumed to be spatial constant but time dependent. The boundary conditions at the outer vessel boundary are given as:

\[
\frac{\partial T}{\partial r} = 0, \quad \frac{\partial Y_i}{\partial r} = 0, \quad v = 0
\]

The droplet surface boundary conditions are based on mass, species and energy flux continuity and on fugacity equilibrium.

The grid applied in liquid phase is linear while that one in the gas phase is an exponential one. Calculation will continue after the droplet has vanished that is when its diameter has become sufficiently small to be regarded as zero. From this time only the gas phase will be calculated and symmetry conditions will be applied at the former droplet surface.

As mentioned in \(^2\) this model can directly be compared to a uniform mono-disperse spray. Where the ratio of the initial droplet diameter and of the (constant) vessel diameter gives the overall equivalence ratio \( \Phi \) and thus is a measure for the density of the droplets.

For this study the reduced kinetic with 437 and 92 species\(^1\)\(^2\) is used which has already validated through the comparison with experiments (micro gravity and 1g)\(^2\).

Ignition is defined as the moment the temperature of 1300 K is reached at any point in the gas phase.

The initial temperature of the droplet is varied from 280 K to 313 K. The gas temperatures for this study are 750 K and 800 K.

5. Results

The experimental results for induction time against Temperature are shown in Fig. 5 for all fuel temperatures.

As can be seen there is a large variation of the induction times, but there is still a trend visible, showing an expected reduction in induction time with higher temperature. Due to these variation it is not possible to make out a difference between the trends for individual fuel temperatures.

In addition to this an uncertainty zone was defined. Within this temperature range not all sprays ignited, this is most probably due to random events in the spray (such as turbulence) and this phenomenon is currently being investigated further.

If one now separates out individual fuel temperatures the variations become much less severe as can be seen in Fig.6. There is however still a fair variation, which can be due to several factors. One could be the uneven injection of the fuel, which will be a technological factor that could be reduced. This is currently being investigated. However there are also other hypotheses such as the above mentioned random events that are always present in a spray and could lead to the variations in induction times.

![Fig. 5 Induction times all fuel temperatures](image)

![Fig. 6 Induction times fuel 293 K](image)
Nonetheless it was possible to compare the experimental results with the numerical ones and obtain an interesting parameter space; this can be seen in Fig. 7 through Fig. 10.

The shaded areas show where the numerical results of a mono disperse equidistant spray coincide with the experiments of a real spray. The upper and lower lines represent the maximum and minimum induction times measured for the experiments (and hence show the variation), while vertical boundaries for this area are an arbitrary ±10µm variation in SMD.

If one now remembers the estimated value of $\phi = 0.45$ it can be clearly seen that all shaded areas of the comparison lie within about this range. It is also interesting to note that a higher fuel temperature seems to induce an ignition of leaner fuel air mixtures, as the shaded area shifts slightly into the leaner region albeit at the cost of slightly longer induction times.

This shows that it might be possible to describe some of the behaviour of a real spray with the simulation of a mono dispersed equidistant spray. However, further narrowing down of the experimental parameters will be necessary (and ongoing) to confirm this hypothesis.

6. Conclusion

This paper described the first attempt by the ZARM combustion group to simulate some of the behaviour of a real spray by simulating a mono dispersed equidistant spray with the closed vessel code.

It was shown that a combined parameter space exists and that some of the behaviour of the spray might be described in this fashion, however further work in narrowing down the experimental parameters as well as further simulations will be needed to give a more complete picture.

The results represent a building block toward a more advanced and complex model.

7. Acknowledgements

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References

