# Interpretation of Auto-ignition Delay Times Measured in Different Rapid Compression Machines

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#### **1** Introduction

An international collaboration was initiated by thirteen different research groups to understand and explain the differences in auto-ignition delay times, measured on different rapid compression machines, RCMs, of different design and size [1,3]. The Consortium measured delay times,  $\tau$ , for *i*-octane under the same conditions: fixed oxygen content of 21%, pressure at the end of compression,  $P_o$ , 2.0 MPa, and compression temperatures,  $T_o$ , in the range 650-950K. Figure 1 gives the experimental auto-ignition delay times,  $\tau_e$ , from seven different RCMs plotted against  $1000/T_o$ . Each point is identified by a number unique to each participating group. There is significant scatter in  $\tau_e$ , particularly at the intermediate and low temperatures.



Figure 1. Auto-ignition delay times,  $\tau_e$ , of stoichiometric iso-octane from the different RCMs, plotted against end of compression reciprocal temperature  $T_o (P_o \sim 2.0 \text{MPa})$  [2].

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Pressure records for three of the machines, 1, 5, and 6, for similar pressure conditions are shown in Fig. 2. Values of  $T_o$  are given for each compression and the measured delay times,  $\tau_e$ , are differences between the times at *i* and *o*,  $t_i$  and  $t_o$ . Clearly, the machines have different values of  $\tau_e$ . Reasons for these differences include (i) heat loss after compression, (ii) reaction during non-instantaneous compression (iii) possible piston bounce and non-uniform ignition, among others.



Figure 2. Pressure traces for RCMs 1, 5, and 6 at end of compression conditions ( $P_o \sim 2.0$ MPa,  $T_o = (790$ K-797K))

## 2 Effects of heat loss

During the cooling and possible heat release following compression, the temperature of the adiabatic core, T, is determined from the measured pressure, P, using the isentropic law:

$$\frac{T}{T_o} = \left(\frac{P}{P_o}\right)^{\frac{\gamma-1}{\gamma}},\tag{1}$$

where  $\gamma$  is the ratio of specific heats for the mixture.

Pressure and temperature are continually changing and, to allow for this, a temporal mean temperature is given by:

$$T_{m} = \frac{1}{t_{i} - t_{o}} \int_{t_{o}}^{t_{i}} T dt , \qquad (2)$$

and a mean pressure similarly, by:

$$P_{m} = \frac{1}{t_{i} - t_{o}} \int_{t_{o}}^{t_{i}} P dt , \qquad (3)$$

The original experimental delay time  $\tau_e$  is then attributed to  $T_m$  and  $P_m$ , rather than  $T_o$  and  $P_o$ . Leakage from the cylinder and combustion chamber is assumed to be negligible.

The measured delay times,  $\tau_m$ , now associated with  $T_m$  and  $P_m$ , following convention, should be attributed to the values at the end of compression,  $T_o$  and  $P_o$ . The influence of this pressure change on  $\tau$  was expressed by an inverse pressure proportionality,  $P^n$ , employing values of *n* from [4], while the influence of temperature was expressed by:

$$\tau \alpha \exp\left(\frac{E}{RT}\right),$$
 (4)

Localised values of E/R, the activation temperature, were found, iteratively, initially by differentiating the values of  $\tau_m$  after applying the pressure correction, with respect to inverse of  $T_m$ , using:

$$\frac{E}{R} = \frac{d \ln \tau_m}{d(1/T_m)},\tag{5}$$

Values of the revised delay time,  $\tau_o$ , in terms of  $P_o$  and  $T_o$ , were found using *n* and *E/R* in the expression:

$$\tau_o(P_o, T_o) = \tau_m \left(\frac{P_o}{P_m}\right)^{-n} \exp\left(\frac{E}{R}\left(\frac{1}{T_o} - \frac{1}{T_m}\right)\right),\tag{6}$$

The resulting values of  $\tau_o$  for the seven different RCMs are plotted against  $1000/T_o$  in Fig. 3. It can be seen that the scatter, particularly in the negative temperature coefficient, NTC, region, has been reduced.



Figure 3. Corrected delay time,  $\tau_o$ , of stoichiometric iso-octane for  $T_o$ , and  $P_o = 2.0$  MPa.

### **3** Effects of reaction during compression

The pressure traces in Fig. 2 show clearly the variations in the times of compression for the different RCMs. Data for the effects of this upon reaction, prior to attaining  $P_o$  were sought through evaluation

of the Livengood-Wu integral, LWI, for the duration of the compression. This is an integration of the reciprocal ignition delay time with regard to time, under the changing conditions of the compression:

$$\int_{t_s}^{t_o} \frac{dt}{\tau(P,T)} = (LWI)_o , \qquad (7)$$

where  $t_s$  and  $t_o$  are the time at the start and end of compression, respectively.



Figure 4. Calculated (LWI)<sub>o</sub> for different RCMs at selected temperatures  $T_o$ ,  $P_o=2.0$  MPa.



Figure 5. Derivation of  $\tau_c$  from  $\tau_o$  by extrapolation to (LWI)<sub>o</sub>=0 for different RCMs, at different  $T_o$ ,  $P_o$ =2.0 MPa.

Shown in Fig. 4 are plots of  $(LWI)_o$  for the different RCMs, against  $1000/T_o$ . Values of  $t_{50}$ , the time from  $0.5P_o$  to  $P_o$ , also are given. Values of  $(LWI)_o$  increase with increases in  $T_o$ , and reaction rate, as well as in  $t_{50}$ . Values of  $\tau_o$  for each RCM from Fig. 3 were plotted against their corresponding values

of (LWI)<sub>o</sub> from Fig. 4, for different values of  $T_o$ . Figure 5 shows some typical value of such plots over a restricted range of  $T_o$ .

Ideally, the compression should be instantaneous, in which case (LWI)<sub>o</sub> would be zero. Consequently, in such figures, the values of  $\tau_o$  are extrapolated to give a corrected value at (LWI)<sub>o</sub> = 0, namely  $\tau_c$ . These "corrected" values  $\tau_c$ , are plotted against 1000/ $T_o$  by the full line curve on Fig. 6. The symbols indicate the originally measured RCM values.



Figure 6. Continuous curve shows derived ideal "corrected" values of ignition delay times,  $\tau_c$ , for stoichiometric iso-octane at the measured  $T_o$  and  $P_o=2.0$  MPa. Symbols show original measured points,  $\tau_e$ .

### 4 Overall Livengood–Wu integral and severity of auto-ignition

The derived values of  $\tau_c$  and the associated experimental pressures and temperatures for the different RCMs, were employed to evaluate the Livengood-Wu integral (LWI)<sub>i</sub>, from the experimental start of compression time  $t_s$  up to the auto-ignition point *i*,  $t_i$ , on Fig. 2. Values of the integral for the different RCMs are shown by the symbols on Fig. 7. The best curve fit through the data points has values close to unity, with a trend of falling below unity at the highest temperatures. The dashed curves show the upper and lower limits of the integral when the original experimental values,  $\tau_e$ , were employed in the evaluation, indicating a much greater scatter and departure from unity of the integral. The integral values based on  $\tau_c$  are much closer to unity and this is indicative of improved accuracy.

The integral values fall below unity at the higher temperatures, at which the pressure rises were steeper with pronounced oscillations, not attributable to piston bounce. The higher rate of change of heat release rate generated stronger pressure pulses than in the milder auto-ignition at the lower temperatures [5-7].

## 5 Conclusion

The diversity of the different RCMs has been advantageously utilised to increase our understanding of the departures of the RCMs from their ideal performance. It is emphasised that the performances of all the RCMs are those at the time that the data was submitted to the Consortium. They are no guide to their present performance at the different centres. Allowances have been made for the effects of reaction during compression and heat loss thereafter. At the higher temperatures, stronger auto-ignition occurs at reactive hotspots, reducing the overall Livengood-Wu integral. Considerations of

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these factors have made it possible to derive values of auto-ignition delay times that are probably more accurate.



Figure 7. Calculated (LWI)<sub>*i*</sub> values using the original experimental temperatures and pressures in the different RCMs, but with the associated derived values,  $\tau_c$ . Broken curves show the upper and lower limits of the integral when the original experimental values,  $\tau_e$ , were employed in the evaluation.

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