Auto-ignition Prediction During Hot Start Conditions

J. Wodausch[a,b], *J. Momberg*[b], *J. Roux*[b]
H. Holdack-Janssen[c,d] *and T. van Niekerk*[d]

This paper describes the development of an empirical thermodynamic single-zone model to predict auto-ignition in an internal combustion engine. In this case the development basis is a 1.4 L multi port injection (MPI) internal combustion engine. A model was created to calculate the probability of auto-ignition with regards to the engine design, thermodynamic laws and the carburetion of the air-fuel mixture. The theoretical model developed was verified with measurements. Adequate correlation between the predicted and measured probability results was obtained.

Additional Keywords: Knock detection modelling

Nomenclature
Roman
CB	combustion beginning [˚CA]
CE	combustion end [˚CA]
h	enthalpy [kJ/kg]
I	integral ignition delay factor
K	knock assessment factor
KHB	knock occurance range [˚CA]
m	mass [kg]
MB	mass fraction burnt
n	engine speed [rpm]
p	(measured) in-cylinder (combustion) pressure [Pa]
Q	energy [kJ]
R	universal gas constant [kJ/kg K]
T	in-cylinder temperature [K]
u	enthalpy [kJ/kg]
V	calculated displacement volume [m³/˚CA]
X	knock probability [%]

Greek
α	specific crank angle [˚]
κ	isentropic exponent (1.33)
λ	combustion chamber air-fuel ratio
φ	crank angle [˚]

Subscripts
B	burnt fuel
E	exhaust, knock assessment
I	inlet
K	knock
max.	maximum
min.	minimum
prob.	propability
ref.	reference
SHP	start of high pressure phase
SK	start of knock
W	wall

a   2C Schreberweg, 38108 Braunschweig, Germany
    E-mail: Jens.Wodausch@gmx.de , Tel.: +49 (0)531-3172408
b   Volkswagen, Product Engineering, Uitenhage, South Africa.
c   University of Applied Sciences Braunschweig/ Wolfenbüttel,
    Institute of Vehicle Engineering Wolfsburg, Germany.
    E-mail: Hinrich.Holdack-Janssen@nmmu.ac.za
d   MSAIEE, Nelson Mandela Metropolitan University,
    Department of Mechatronics, Port Elizabeth, South Africa.
    E-mail: Theo.vanNiekerk@nmmu.ac.za

1. Introduction

Computer based simulation of the thermodynamic processes in an internal combustion engine have assisted engine designers for more than 25 years now. It saves time and therefore costs since less testing is necessary. This paper describes the development of a simulation model which predicts auto-ignition during hot start conditions. The point at which auto-ignition will appear is very important because it influences significantly the effective engine efficiency. The challenge is to achieve results close to the optimum efficiency. The model developed will assist the application of the engine maps for the 1.4 L MPI engine in the electronic control unit.

The principle guides for the model development were the dissertation by Franzke[1] and the research report by Spicher and Worret[2, 3]. In his dissertation Franzke used an integral ignition delay to describe the processes in the end-gas mixture. On the basis of the investigations of Franzke and Spicher and Worret, the integral ignition delay is also used to calculate knock probability in this case. The momentary ignition delays, relative to temperature and pressure during compression and combustion, will be integrated for every degree of crank angle. The integral, linked to proportional factors such as temperature and pressure, is an indicator of the concentration of reaction determinant intermediate products in the end-gas mixture. Franzke chose I_K[1, 4] to describe this pre-reaction condition. This paper uses the same nomenclature. The pre-reaction situation when auto-ignition starts is critical.

During compression and combustion the concentration of the reaction determinant semi-finished products increases until they reach a critical value. This value determines when auto-ignition will occur in the end-gas mixture.

2. Combustion Analysis

Combustion analysis yields important information about engine operation and is necessary for further investigations (e.g. knock prediction). In detail, the heat release per degree crank angle and the percentage of the mass fraction burnt will be calculated. Four different points are significant for the assessment of combustion behaviour. Combustion starts at 1 % and normally ends at 95 % mass fraction burnt. However, Spicher and Worret[2, 3, 5] ascertained that combustion ending at 75 % of the mass fraction burnt has

the accuracy suitable for knock prediction. In this paper combustion duration is defined as being 1 to 75 % mass fraction burnt. The 50 % point (centre of combustion) is used as an indicator to assess combustion and allow a comparison of the different measurements. The centre of combustion should lie at 8° crank angle (CA) after top dead centre (TDC) in an engine operating at constant speed and load[4, 6, 7, 8]. In terms of the first law of thermodynamics, the combustion chamber is an open system. In this system different events occur per degree crank angle. Figure 1 shows the input and output quantities of the combustion chamber.
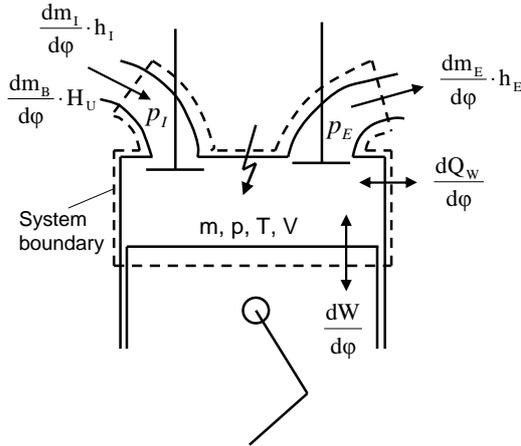

Figure 1: First law of thermodynamics (open system)[7, 9]

Heat release in the combustion chamber is calculated from an energy balance. The energy balance for an open system, with reference to figure 1, is given as:

$$\frac{d\left(m \cdot u\right)}{d\varphi} = \frac{dQ_B}{d\varphi} + p \cdot \frac{dV}{d\varphi} + \frac{dQ_W}{d\varphi} + \frac{dm_I}{d\varphi} \cdot h_I + \frac{dm_E}{d\varphi} \cdot h_E \qquad (1)$$

where:

$\dfrac{d\left(m \cdot u\right)}{d\varphi}$ = change in internal energy [kJ/°CA]

$\dfrac{dQ_B}{d\varphi}$ = input fuel energy [kJ/°CA]

$p \cdot \dfrac{dV}{d\varphi}$ = work per crank angle [kJ/°CA]

$\dfrac{dQ_W}{d\varphi}$ = heat transfer to the cylinder [kJ/°CA]

$\dfrac{dm_{I,E}}{d\varphi} \cdot h_{I,E}$ = inlet/ exhaust mass flow [kJ/°CA]

The following assumptions by Manz[8] with reference to Hohenberg are adopted in this paper to calculate the heat release to mass fraction burnt ratio. The heat transfer to the cylinder wall is zero during the heat release calculation.

$$\frac{dQ_W}{d\varphi} = 0 \qquad (2)$$

Mass flow is zero due to the fact that only the high pressure phase is investigated.

$$\frac{dm_{I,E}}{d\varphi} \cdot h_{I,E} = 0 \qquad (3)$$

The air-fuel ratio (λ) in the combustion chamber is homogenous.

$$\frac{d\lambda}{d\varphi} = 0 \qquad (4)$$

The ideal gas law is valid (R = constant). Taking into consideration these assumptions, using the ideal gas law, the heat release [kJ/°CA] equation is simplified to:

$$\frac{dQ_H}{d\varphi} = \frac{1}{\kappa - 1} \cdot \left(\kappa \cdot p \cdot \frac{dV}{d\varphi} + V \cdot \frac{dp}{d\varphi} \right) \qquad (5)$$

Mass fraction burnt is the integral of the heat release calculation. This result is scaled to 100 % and shows the progress of combustion accordingly. At the ignition point (6° before TDC), 0 % of the mass fraction is burnt and it is assumed that at the end of the calculation (360°CA), 100 % of the mass fraction is burnt. These conditions are the calculation limits for the integral. Merker[10] recommends the following equation to calculate the combustion progress:

$$MB = \int_{CB}^{CE} \left(\frac{dQ_B}{d\varphi} \right) \cdot d\varphi \qquad (6)$$

where

$\dfrac{dQ_B}{d\varphi}$ = heat release [kJ/°CA]

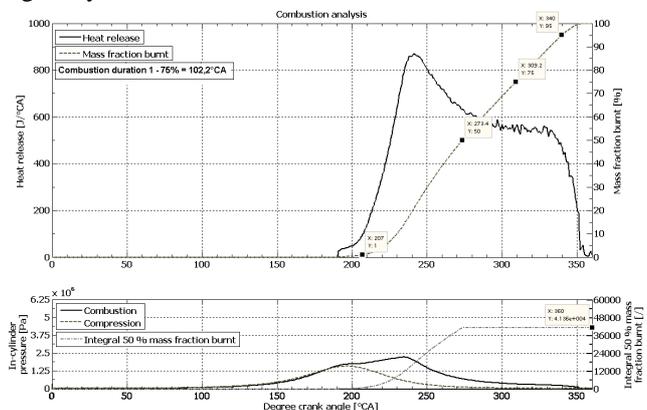Figure 2 shows the calculation result from a non-knocking engine cycle:

Figure 2: Combustion analysis for a non-knocking engine cycle

3. Knock Criterion

The calculation of the auto-ignition point is based on the integral ignition delay time. The critical pre-reaction value (starting point of auto-ignition) occurs when the result of equation 7 equals one. The associated angle is α_K relative to degree crank angle. The following equation was used to calculate the integral ignition delay[2] (I_K):

$$I_K = \frac{1}{6 \cdot n} \cdot \left(\frac{1}{2.37 \cdot 10^3} \right) \cdot \int_{\varphi_{SHP}}^{\varphi_{SK}} p^{1.299} \cdot e^{\frac{4179}{T}} \, d\varphi \qquad (7)$$

Figure 3 below shows the result for the integral ignition delay calculation for the heat release curve presented in figure 2:
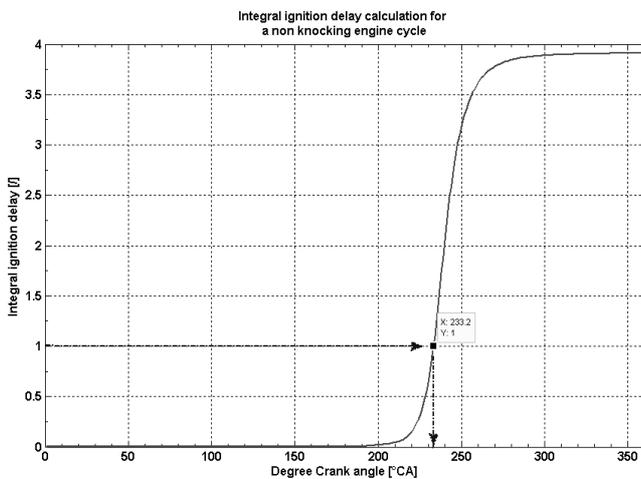

Figure 3: Integral ignition delay

The factor I_K shows at which point the critical pre-reaction value for the start of knock would theoretically be reached ($I_K = 1$). Franzke's investigations showed that auto-ignition would not necessarily always occur at this point. In this case figure 3 shows a definite non-knocking measurement. It introduces the K-factor which leads to another angle α_E. This angle must be compared to α_K and only then a prediction of knock probability is possible. The relationship between the different angles will be explained in section 4.

4. Crankshaft Angle α_E

The integral ignition delay factor I_K shows when the air-fuel mixture will achieve its critical pre-reaction level and leads to the angle α_K. On the basis of global flame propagation, Franzke[1] developed a second assessment factor $K_{ref.}$ which leads to the angle α_E. Both these angles, in relation to each other, provide evidence of knock probability. Calculation of the assessment factor $K_{ref.}$ requires a measurement of auto-ignition which will be used as a reference. The important values needed to calculate this reference factor will be obtained from a reference measurement in which there was audible knock and substantial pressure oscillation. The following equation will be used to calculate the angle α_E:

$$\alpha_E = K_{ref.} \cdot (CE + CB) + CB \qquad (8)$$

The results from equations 7 and 8 yield the required angles α_E and α_K.

5. Probability K_W

The equations calculate crank angle positions relative to the critical pre-reaction situation and the characteristic crank shaft angle. These two angles relative to each other provide evidence of knock probability. Spicher and Worret[2] investigated approximately 400 measurements and found that I_K and $K_{ref.}$ values were repeatable over a measured range. They decreased this range for I_K to 15 % and $K_{ref.}$ to 5 % during their investigations. Consequently this means that every angle has a lower and an upper limit. Due to the position of α_E and α_K it is therefore possible to formulate a logical inter-dependency to describe knock probability. The different input signals cause different results and in this case different angle positions. Figure 4 illustrates the relationship:
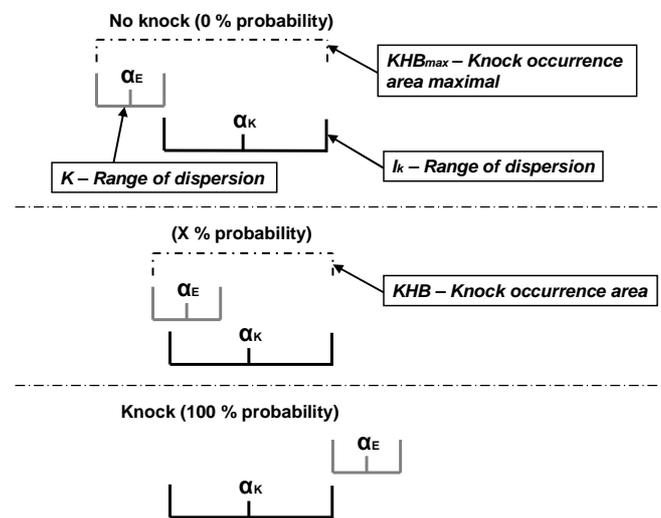

Figure 4: Knock probability vs. the angles α_E and α_K [2]

The two principal limits for the inter-dependency are 0 and 100 % probability. The 0 % probability occurs when the angle α_{Kmin} is in front of α_{Emax}. The ranges do not overlap and therefore, with reference to Spicher and Worret, auto-ignition[2, 3] is impossible. When α_{Kmax} is behind α_{Emin} the probability is 100 % and auto-ignition will definitely happen. The probability is 50 % when the angles α_E and α_K are the same. The probability is 100 % when

$$\frac{KHB}{KHB_{max.}} \leq 0 \qquad (9)$$

because KHB will be zero and therefore the result is zero.

$$KHB_{max.} = \Delta\alpha_E + \Delta\alpha_K \qquad (10)$$

$KHB_{max.}$ remains constant and can be calculated from the intervals of α_E and α_K.

$$\Delta\alpha_E = \alpha_{E\,max.} - \alpha_{E\,min.} \qquad (11)$$

$$\Delta\alpha_K = \alpha_{K\,\text{max.}} - \alpha_{K\,\text{min.}} \qquad (12)$$

The probability is 0 % when

$$\frac{KHB}{KHB_{\text{max}}} \geq 1 \qquad (13)$$

because KHB becomes greater than KHB_{max}, which can have only the value of the accumulated intervals. Equation 9 indentifies the range in which equation 10 will be used to calculate the probability between 0 and 100 % with the assumption of linear dependency.

$$\left(0 < \frac{KHB}{KHB_{\text{max.}}} < 1\right) \qquad (14)$$

$$X_{\text{prop.}} = -100 \cdot \frac{KHB}{KHB_{\text{max.}}} + 100 \qquad (15)$$

6. Verification

The results from the pre-investigations showed that an additional adaption factor is necessary to adjust the value of the angle α_E. This adaption factor is linked to the peak heat release measurements at different calibration levels and conditions during start. Four points were investigated in detail to obtain such appropriate adaption factors. These points are:

❑ Cold Start
❑ Hot start with old calibration level
❑ Hot start with new calibration level
❑ Hot start with severe auto-ignition during start

The cold start analysed shows a peak heat release of about 870 J/°CA without auto-ignition. Due to the fact that the entire engine is cold, the engine is less likely to knock during start because the air-fuel mixture cannot exceed the spontaneous ignition temperature. As a result the probability for auto-ignition must be 0 % i.e. the adaption factor must move the position of α_E until α_{Emax} and α_{Kmin} are almost equal.

The analyses of hot starts with the new calibration level show an average peak heat release of 915 J/°CA. This value is greater than the peak heat release from the cold start analysed. The investigations showed that the calibration changes minimized auto-ignition during start but the engine was still very hot. There is a small probability of spontaneous ignition of the air-fuel mixture in the combustion chamber. The probability for this type of start was set to 20 % because auto-ignition is still possible but less likely. Therefore the position of α_E was modified by the adoption factor until equation 15 delivered the expected probability.

Analysis of the measurements with the old calibration level showed an average peak heat release of 1070 J/°CA. Auto-ignition appeared almost during every hot start. The

expected knock probability was therefore set to 80 % and the adoption factor modified accordingly.

Only measurements with severe auto-ignition were used for analysis of the 100 % knock probability point. The average peak heat release for these points is 1409 J/°CA. Correspondingly the adaption factor was modified to achieve a probability of 100 % with equation 15. That means in this case the position of α_E must be moved until $\alpha_{Emin.}$ and $\alpha_{Kmax.}$ are almost equal. Analysis of combustion showed that a connection between the adaption factor for α_E and the peak heat release exists. The lowest adaption factor (1.01064) is necessary for a cold start to reach 0 % probability and the highest adaption factor (1.05826) for 100 % probability. The 20 and 80 % adaption factors lie between these two values. Figure 5 clarifies these results and shows the average value of the peak heat release (x-axis) for the measurements printed over the adaptation factor (y-axis):

A small peak heat release (cold start) requires a small adaptation factor and a greater peak heat release (old calibration level/always auto-ignition) requires a greater adaptation factor i.e. the worse the start the higher the adaptation factor. The assumed linear dependency enables the calculation of the adaptation factor as a function of the peak heat release which will be obtained from the combustion analyses. The theory developed (adaptation of the angle α_E) was verified by measurements. Table 1 shows the probability for the adaptation of the characteristic crank angle α_E.
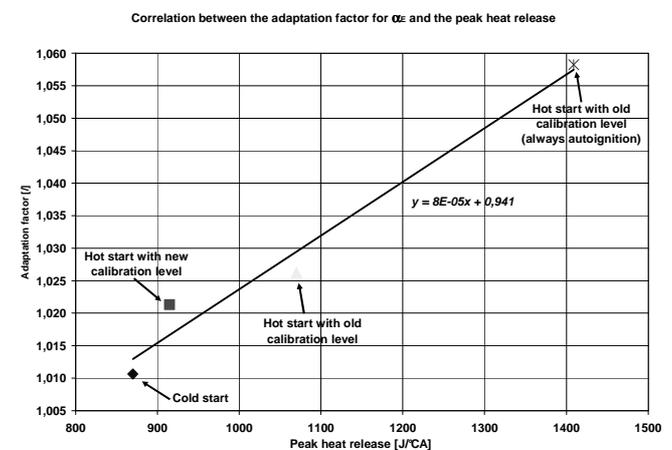

Figure 5: Adaptation factor for α_E vs peak heat release

Random data sets from measurements with the old calibration level were used for the probability verification. The combustion analysis shows a peak heat release between 1160 and 1200 J/°CA and peak pressure of between 49 and 52 bar. The high value of the peak heat release shows that a high quantity of fuel is available in the combustion chamber. The adaptation factor calculated lies between 1.0338 and 1.0370, depending on the peak heat release. Consequently the knock probability is between 77.9 and 85.7 %. These results are realistic due to the high peak heat release of the measurements analysed.

7. Summary

The focus in this paper is the prediction of auto-ignition. A simulation model was built and configured to calculate knock probability for a 1.4 L engine during hot start. Different steps in the analysis are necessary to accumulate the required data e.g. a combustion analysis provides information about the peak heat release and the mass fraction burnt. This information is used to calculate the integral ignition delay, characteristic crankshaft angle and probability. The probability calculation is based on a linear equation which was developed in this paper.

	Measurement 1	Measurement 2	Measurement 3
Angle α_K [°CA]	228,0	227,0	230,0
$\alpha_{Kmax.}$ [°CA]	255,5	251,5	254,5
Angle α_K with regard to the reference TDC 239°CA [°CA]	253,0	249,0	252,0
$\alpha_{Kmin.}$ [°CA]	250,5	246,5	249,5
Delta α_K [°CA]	5,1	5,0	5,0
Original angle α_E [°CA]	247,5	243,4	246,3
$\alpha_{Emax.}$ [°CA]	258,5	253,9	257,7
Angle α_E adapted with factor [°CA]	256,2	251,7	255,4
$\alpha_{Emin.}$ [°CA]	253,9	249,4	253,1
Delta α_E [°CA]	4,6	4,5	4,6
Offset factor for α_E [/]	1.0354	1.0338	1.0370
KHB [°CA]	1,6	2,1	1,4
KHB$_{max.}$ [°CA]	9,7	9,5	9,6
Combustion duration [°CA]	95,4	88,5	88,5
Peak heat release [J/°CA]	1180	1160	1200
Probability [%]	**83,5**	**77,9**	**85,7**

Table 1: Knock probability calculated with adapted angle α_E

8. Conclusion

The probability results show adequate correlation between the calculated and expected results derived from the measurements which were used for verification.

9. Acknowledgments

References

1. *Franzke D*, Beitrag zur Ermittlung eines Klopfkriteriums der ottomotorischen Verbrennung und zur Vorausberechnung der Klopfgrenze, Dissertation, Fakultät für Maschinenwesen, University of Munich, 1981.
2. *Spicher U and Worret R*, Entwicklung eines Kriteriums zur Vorausberechnung der Klopfgrenze, final research report, Institut für Kolbenmaschinen, University of Karlsruhe, 2001.
3. *Spicher U and Rothe M*, Extremklopfer – Ursachenforschung nach schadensrelevanten klopfenden Arbeitsspielen, final report, Institut für Kolbenmaschinen, University of Karlsruhe, 2005.
4. *Heywood, JB*, Internal Combustion Engines Fundamentals, McGraw-Hill Book Company, Massachusetts Institute of Technology, 1988.
5. *Küntscher V and Hoffmann W*, Kraftfahrzeugmotoren, Vogel publishing company, fourth print run, Würzburg, 2006.
6. *Basshuysen R and Schaefer F*, Lexikon Motorentechnik, Vieweg publishing company, first print run, Wiesbaden, 2004.
7. *Basshuysen R and Schaefer F*, Handbuch Verbrennungsmotor, Vieweg publishing company, second print run, Braunschweig/Wiesbaden, 2002.
8. *Manz PW*, Indiziertechnik an Verbrennungsmotoren, lecture notes, Fakultät für Maschinenbau, University of Braunschweig, 2008.
9. *Cerbe G and Wilhelms G*, Technische Thermodynamik, Carl Hanser publishing company, 14 print run, Munich, 2005.
10. *Merker G, Schwarz C, Stiesch G and Otto F*, Verbrennungsmotoren Simulation der Verbrennung und Schadstoffbildung, Teubner publishing company, third print run, Wiesbaden, 2006.