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COLDSTART ENGINE COMBUSTION MODELLING TO CONTROL HYDROCARBON EMISSIONS

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Abstract:
Due to the large contribution of the coldstart process to unburned hydrocarbon emissions of an internal combustion engine during FTP cycle tests, we take a new look at the production of hydrocarbons inside the combustion chamber during coldstart. To this end a model is developed which predicts the exhaust port hydrocarbon concentration, exhaust gas temperature and equivalence ratio based on a simplified, control-oriented heat release analysis of the cylinder pressure. Non-linear control algorithms are used to regulate the engine to a pre-defined exhaust profile, based on optimized catalyst-out hydrocarbon emissions. This approach is intended to make use of robust, automotive-grade exhaust hydrocarbon sensors currently in development.

Keywords: Automobiles, Air Pollution, Automotive Emissions, Automotive Control, Control Oriented Models, Engine Modelling, Engine Management, Non-linear Models, Spark Advance Control

1. INTRODUCTION

Hydrocarbon emissions from engines have been regulated since initial legislation was passed in the late 1950's. Throughout the 1970's and 1980's, the catalytic converter was introduced and refined to a state such that the vast majority of all regulated pollutants, Hydrocarbons (HC), Carbon Monoxide (CO), and Nitrogen Oxides (NO_x), are removed from the engine exhaust by reduction or oxidation, resulting in a much cleaner exhaust stream from the automobile. However, the catalyst used in conventional automobiles is not active below temperatures of around 400C, resulting in large amounts of pollution during the coldstart phase of operation, generally speaking the first 120 seconds of operation, especially HC emissions. This is further complicated by the adverse operating conditions of the engine, including cold combustion chamber walls and poor vaporization of fuel, resulting in large heat transfer losses to the engine housing and over-rich concentrations of fuel in the combustion chamber that escape the engine unburned. An additional constraint is the fact that the main sensor used for feedback control of automotive spark-ignition engines is the Oxygen sensor, which is also not active at cold temperatures.

This paper focusses on the development of an engine model that could be used in a control strategy based on feedback of the HC emissions from the engine, either directly using newly developed exhaust hydrocarbon sensors, or indirectly via heat Release analysis, based on cylinder pressure measurement. The pollutant of interest in this research is unburnt hydrocarbons, as it has been shown that over 90% of the HC emissions from an automobile are emitted during the coldstart period.

2. COLD START ENGINE COMBUSTION MODEL

The fundamental model of hydrocarbon emissions production in the spark-ignition engine is centered around a Heat Release analysis technique in common use around the world in the field of engine combustion diagnostics and development. However, its use has not seen widespread use in the area of engine Control.

The model begins with a control volume around the combustion chamber and employs the 1^{st} law of thermodynamics to arrive at the following relationship for heat release during combustion

$$\delta Q_{hr} = \delta U + \delta Q_{ht} + \delta W \tag{1}$$

where δQ_{hr} is the heat release due to conversion of fuel, δU is the sensible energy $= mc_v(T)dT$, and δW is the work output from the combustion event $= PdV$.

It is extremely important to state that one can NOT neglect heat transfer here. In many efforts that have been presented as well as established engine analysis techniques, the first approximation made is to neglect heat transfer. This approximation would only be valid during fully warmed-up, thermal steady state conditions. This is clearly not the case during coldstart.

The heat release is thus expanded as:

$$\delta Q_{hr} = (\frac{c_v}{R})VdP + (\frac{c_p}{R})PdV + h_c A(T - T_w)dt \tag{2}$$

2.1 *Combustion Heat Transfer Model*

An essential component of a model describing the coldstart emissions behavior of an internal combustion engine is the mechanism of heat transfer to the relatively cold engine walls from the hot combustion gases. Because the emissions behavior of the engine changes drastically with operating temperature, the heat transfer mechanism can not be neglected during the coldstart period.

2.1.1. *State of the Art* There is very little in the literature in the way of heat transfer modelling that is applicable to realtime control of internal combustion engines. As a result, most engine modelling research presented can be categorized into two general areas.

The first area is that of detailed, often finite element-based, modelling of the combustion process that is typically run on the fastest computer available. The computation time required for a single cycle analysis exceeds the duration of the combustion event by several orders of magnitude. This type of modelling, although quite accurate, is clearly not suitable for control purposes.

Engine models developed for control purposes almost universally neglect the heat transfer losses in the combustion chamber as the first approximation. These types of models are only applicable during thermal steady-state operation and are of limited use in describing or controlling operating conditions involving large temperature transients such as the coldstart process. Some models are augmented by empirically derived constraints to overcome the initial cold operation of the engine. These constraints most often involve extensive laboratory and dynamometer testing and calibration before they can be put into practice.

This can be attributed to a number of reasons, primarily the difficulty of computation of multi-dimensional, coupled partial differential equations describing the heat transfer in an internal combustion engine. The advent of "super-computing" capabilities at the personal computing level that increase naturally according to Moore's law has greatly reduced the time and effort required to perform numerically intense calculations of reacting flow dynamics inside the combustion chamber. However, we are unable to overcome the inherent iterative and recursive nature of such calculations that inhibit their use in a control scenario. A difficulty faced by current control-oriented models is the extreme complexity of the heat transfer process and the inability to directly measure, in any robust and cost-effective manner, the requisite operating parameters of an internal combustion engine. This is coupled with the relative lack of experience with any sort of generalized engine warmup and heat exchange behavior.

Therefore there is still a definite need for accurate, simplified models describing the heat transfer process that can be applied towards the development and implementation of model-based realtime control. It is the intent of the research to define such a model that accounts for the heat transfer loss in the combustion chamber and its subsequent effect on engine emissions.

2.1.2. *Heat Transfer Correlations* The most widely cited heat transfer correlation in the literature is attributed to (Woschni, 1967). In this seminal work, a generalized relationship for heat transfer losses to the combustion chamber walls during combustion that is universally applicable to all types of internal combustion engines is developed. The relationship for the heat transfer, h_c,

$$h_c = CB^{m-1}P^m w^m T^{(0.75-1.62m)} \tag{3}$$

where w = average gas velocity $\propto$ mean piston speed, C = some constant, B = cylinder bore, and m = empirically determined from many engines $\approx$ 0.8, is generally applied to many different engine configurations with good results. However, it is worthwhile to take a closer look at the correlation and some of the limitations it faces. It is also worth mentioning that this correlation was developed empirically using data from primarily large, low-speed diesel engines.

Much effort has been directed at improving and extending the applicability of the above relationship for heat transfer to the combustion chamber walls, however the general validity has not come into question. One of the more significant variations of this relationship is that of (Hohenberg, 1980). Two notable differences are the use of the diameter of a sphere with volume equivalent to the instantaneous combustion chamber volume as the characteristic length

$$d^{-0.22} = C(V^{0.33})^{-0.22} \tag{4}$$

and a velocity component of the heat transfer dependent on the instantaneous gas temperature as well as the mean piston speed

$$w^{0.78} = \left(T^{0.1625}(c_m + 1.4)\right)^{0.78} \tag{5}$$

leading to the following formulation of the overall heat transfer coefficient for heat transfer to the walls of the combustion chamber:

$$h_c = 130V^{-0.06}p^{0.78}T^{-0.4}(c_m + 1.4)^{0.78} \tag{6}$$

This equation was validated against experimental results from smaller, higher-speed diesel engines typical of automotive use.

A further improvement to these relationships in order to describe better the operation of high speed spark ignition engines was conducted by (Bargende, 1991), resulting in the overall heat transfer coefficient

$$h_c = 253.5V^{-0.073}{T_m}^{-0.477}p^{0.78}w^{0.78}\Delta$$
$$\Delta = \left(X\frac{T_b}{T_g}\frac{T_b - T_w}{T_g - T_w} + (1-X)\frac{T_u}{T_g}\frac{T_u - T_w}{T_g - T_w}\right)^2 \tag{7}$$

where X is the fraction of heat release as a function of crankangle during the combustion event. It is clear from the above relationship that use of a 1-zone combustion model where $T_b = T_u = T_g$ leads to a combustion correction term of $\Delta = 1$.

The remaining terms are computed from:

$$T_g = \frac{pV}{mR} \tag{8}$$

$$T_m = \frac{T_g + T_w}{2} \tag{9}$$

$$w = \frac{\sqrt{8k + {c_k}^2}}{2} \tag{10}$$

where k is the specific kinetic energy of the gas derived from combustion turbulence modelling and c_k is the instantaneous piston speed.

Simplifications to this formulation for control purposes tends to a result more closely matching that of Hohenberg. A 1-zone combustion model not incorporating detailed turbulence effects and based on the gas temperature yields, after incorporation of the ideal gas law, the following tractable heat transfer coefficient:

$$h_c = C_1V^{-0.06}p^{0.78}T^{-0.4}(c_m + 1.4)^{0.78} \tag{11}$$

The instantaneous combustion chamber surface area is

$$A = A_h + A_p + A_w + 0.25(2\pi Bh) \tag{12}$$

where A_h is the surface area of the cylinder head, A_p is the surface area of the piston head, A_w is the cylinder wall surface area, and h is the height of the piston crown. This can be further simplified by using an average cylinder wall surface area during the combustion event and neglecting the surface area of the sides of the pistons, as this analysis does not include effects of flow into and out of the crevice volumes of the combustion chamber, resulting in

$$A = A_h + A_p + \bar{A}_w \tag{13}$$

2.2 *Cylinder Wall Temperature Observer*

In order to compute the heat transfer losses from the combustion gases to the combustion chamber walls, we need to know the combustion chamber wall temperature. There is, of course a distribution of temperature at the combustion chamber walls that varies along the radius of the cylinder as well as axially along the cylinder wall. The literature shows a general consensus that employing an averaged cylinder wall temperature, T_w, is valid for the assessment of heat transfer losses in this regime.

However, measurement of this parameter is very hard to do in practice. Although it has been successfully measured in experimental engines employing over 180 individual thermocouples (Bargende, 1991), recent investigations support

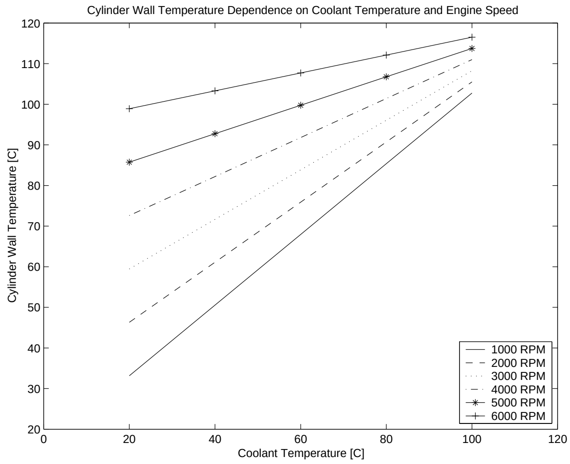

Fig. 1. Dependence of cylinder wall temperature on coolant temperature.

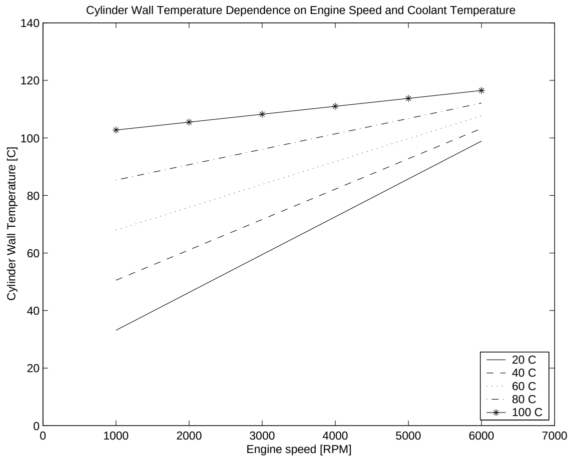

Fig. 2. Dependence of cylinder wall temperature on engine speed.

the measurement of the engine coolant temperature as an accurate indicator of cylinder wall temperature (Halsband, 1994), especially as it pertains to the oil film properties in this region.

Fischer also reports in his analysis of frictional losses in engines that the cylinder wall temperature is primarily dependent on engine speed, engine load and coolant temperature, as well as the position of the piston along its stroke (Fischer, 2000). He further simplifies the dependence of wall temperature on piston position by averaging the temperature over the piston stroke in order to obtain a tractable model of wall temperature.

Linearization of these results over normal operating conditions yields the following relationship for cylinder wall temperature

$$T_w = T_c + (0.945 - 0.0078T_c)\frac{N}{60} + 4.6P_{me} \quad (14)$$

in terms of the coolant temperature, T_c, the engine speed, n, and the engine load, P_{me}.

The dependence of wall temperature on engine speed and coolant temperature at zero load is shown in Figures 1 and 2.

For the purposes of cold start modelling, we are primarily interested in the operating conditions surrounding engine idle and therefore limit the model to an observer based on coolant temperature at a specific load and speed point. The relationship developed is based on data from a specific engine representative of most modern automotive internal combustion engines, however further experimentation on a larger sample set of engines could lead to improved generality of this result.

2.3 *Coldstart Hydrocarbon Formation Model*

In order to model the formation of hydrocarbon emissions from the engine during the coldstart process, we take a close look at the heat release analysis of the engine. Comparison of the actual heat release of the engine observed by direct measurement of the cylinder pressure with the theoretically available heat release results in an estimate of the engine-out hydrocarbon emissions, based on the percentage of unburned fuel emitted from the engine during coldstart.

If we assume a homogeneous mixture in the cylinder and that the quantity $\Delta Q_{hr} = Q_{hr,theor} - Q_{hr,actual}$ is due entirely to unburned Hydrocarbons, or fuel, some of which leaves the cylinder, we arrive at the following analysis:

For lean air/fuel mixtures, the available heat release is computed as

$$Q_{hr,theor} = m_f Q_{LHV} \quad (15)$$

where m_f is the mass of fuel in the cylinder during combustion and Q_{LHV} is the lower heating value of the fuel. This is a measure of the theoretical maximum amount of energy that could be released during combustion.

$$\Delta Q_{hr} = Q_{LHV} m_u \quad (16)$$

where m_u is the mass of unburned fuel in the cylinder

$$m_u = m_f - \frac{Q_{hr,actual}}{Q_{LHV}} \quad (17)$$

$$m_{out} = m_{cyl}(1 - x_r) \quad (18)$$

where x_r is the residual gas fraction in the cylinder. The residual gas fraction can range as high as 20% for spark-ignition engines running at idle, yet a good approximation is:

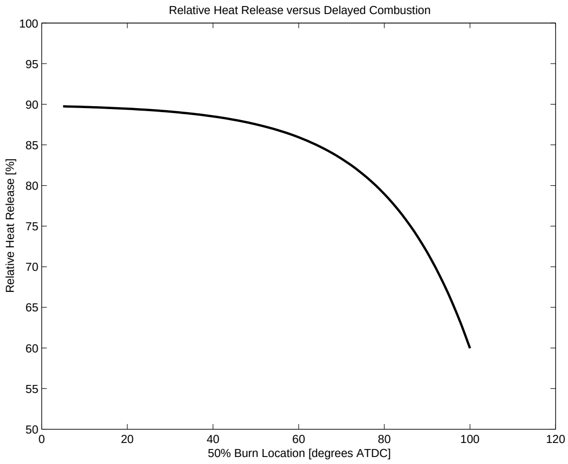

Fig. 3. Relative heat release dependency on delayed combustion.

$$x_r = \frac{m_r}{m} = 1 - \frac{m_a}{m} \approx 1 - \frac{r_c - 1}{r_c} = \frac{1}{r_c} \tag{19}$$

where r_c is the compression ratio of the engine (Heywood, 1988). It is interesting to note here that this assumes that fresh charge fills the displacement volume of the engine and exhaust mixture remains in the clearance volume of the combustion chambers.

This leads to a relation for HC leaving the cylinder as

$$\begin{aligned} m_{HC,out} &= m_u(1 - x_r) \\ &= \left(m_f - \frac{Q_{hr,act}}{Q_{LHV}}\right)\left(\frac{r_c - 1}{r_c}\right) \end{aligned} \tag{20}$$

This assumes the measurement (from cylinder pressure) of Q_{hr}.

This analysis is supported by empirical observations such as that of (Russ, 1999) where it is shown that the total heat release falls to approximately 60% of the available heat release for the cycle, computed using the fuel energy in the cylinder, as the combustion event occurs more slowly and later in the engine cycle. This is due to unburned fuel leaving the combustion chamber and either continued burning or oxidation in the exhaust. The described effect is shown in Figure 3.

2.4 *Cylinder Pressure-based Heat Release Analysis*

The use of measured cylinder pressure to observe net heat release is in common practice today

$$Q_{hr} = \frac{c_v}{R}(PV - P_0V_0) + \int P\frac{dV}{d\theta}d\theta + Q_{ht} \tag{21}$$

$$Q_{ht} = \int Ah_c(T - T_w)\frac{dt}{d\theta}d\theta$$

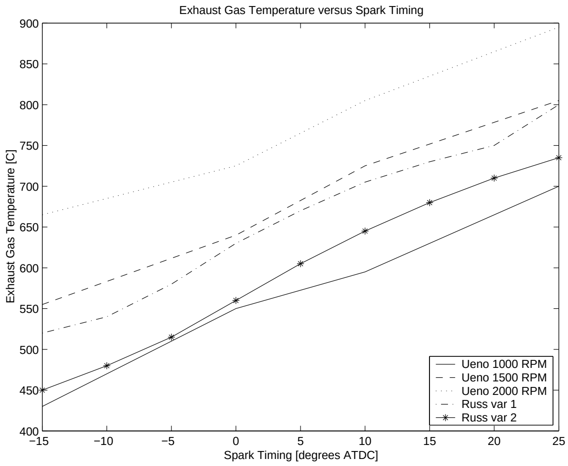

Fig. 4. Linear dependence of exhaust gas temperature on spark timing.

The cylinder gas temperature is estimated from cylinder pressure according to the ideal gas law

$$\begin{aligned} PV &= mRT \\ T_{cyl} &= \frac{PV}{mR} \rightarrow f(\theta) \end{aligned} \tag{22}$$

and it is assumed that the exhaust port gas temperature is roughly equal to the cylinder gas temperature at Exhaust Valve Opening (EVO)

$$T_{exh,EVO} \approx \frac{P_{EVO}V_{EVO}}{mR} \tag{23}$$

2.5 *Spark Timing and Air/Fuel Ratio Effects on Hydrocarbons*

The effect of retarded spark timing on increasing exhaust gas temperature and subsequently reducing tailpipe hydrocarbon emissions is widely reported in the literature (Pozniak, 1976), (Chan and Zhu, 1999), (Russ, 1999), (Ueno, 2000), yet a systematic modelling approach to controlling the spark timing remains to be developed.

Research dating back to 1976 (Pozniak, 1976) clearly shows the effect of retarding spark timing on exhaust hydrocarbons, particularly as they are dependent on exhaust gas temperature. A large body of results show that this effect is, in fact, quite remarkably linear. Recent investigations (Russ, 1999), (Ueno, 2000) extend earlier results to various load and speed points under cold and transient engine operating conditions. A clear linear relationship between spark timing and exhaust gas temperature exists as can be evidenced in Figure 4.

Distillation of these results to the operating conditions under consideration results in the following empirically derived linear relation:

$$T_{exh} = 7.5\Delta ST(CA) + 600\deg C \tag{24}$$

where ΔST is measured in degrees after top dead center, deg $ATDC$.

The mass fraction burned is derived from the commonly-used Wiebe burn profile

$$m_b = 1 - exp\left[-a(\frac{\theta - \theta_0}{\Delta\theta})^m\right] \tag{25}$$

using the normal values of a=2 and m=5 and assuming the parameters are dependent on operating conditions as follows: $\theta_0 \rightarrow f(\Delta ST)$ and $\Delta\theta \rightarrow f(\phi)$. ϕ is the fuel-air equivalence ratio, defined as the current fuel-air ratio divided by the stoichiometric fuel-air ratio, and is the inverse of the industry-preferred expression λ. The actual interaction is in all likelihood much more complex and would require extensive parametric experimentation. This relation is more or less phenomenon-based and not modellable in this approach.

We assume that the ignition delay parameter depends solely on ΔST with good accuracy, as ignition only occurs once the spark has been ignited. This is modelled as a linear function

$$\theta_0 = k_1 \Delta ST + k_2 \tag{26}$$

and the burn duration parameter, $\Delta\theta$, is similarly modelled as a quadratic function of ϕ, which follows intuitively based on the pre-mixed laminar flame speed dependency on ϕ (Kuo, 1986) (Heywood, 1988).

$$\Delta\theta = k3(\phi - \phi_0)^2 + k_4 \tag{27}$$

Ultimately the actual heat release is computed from the mass fraction burned as

$$Q_{hr,actual} = m_b Q_{LHV} \tag{28}$$

3. CONCLUSION

A model has been developed to predict engine-out hydrocarbon emissions based on the available energy release from the amount of injected fuel and the heat transfer losses to the combustion chamber walls during coldstart conditions. The model output is correlated with the actual amount of energy released from the fuel, as determined from heat release analysis via cylinder pressure measurement. Empirical correlations for the effects of spark timing and equivalence ratio are presented, yielding the amount of unreleased fuel energy. This unreleased fuel energy is attributed to unburned hydrocarbons emitted from the engine. The exhaust gas temperature is also estimated based on empirical observations dependent on spark timing.

Further simulation and experimental results are underway to determine the fit of the model to actual operating conditions, leading to the application of a control strategy that can control the exhaust gas composition and temperature. The engine model output is subsequently the input to a thermal coldstart catalytic converter model presented in another paper at this conference. It is the cumulative tailpipe hydrocarbon emissions that must be reduced during the coldstart period, ultimately yielding an engine control algorithm that simultaneously heats the catalyst as quickly as possible while reducing instantaneous hydrocarbons.

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