

Computing Optimal Heat Release Rates in Combustion Engines

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ABSTRACT

The combustion process has a high impact on the engine efficiency, and in the search for efficient engines it is of interest to study the combustion. Optimization and optimal control theory is used to compute the most efficient combustion profiles for single zone model with heat transfer and crevice effects. A model is first developed and tuned to experimental data, the model is a modification of the well known Gatowski et al.-model [1]. This model is selected since it gives a very good description of the in-cylinder pressure, and thus the produced work, and achieves this with a low computational complexity. This enables an efficient search method that can maximize the work to be developed. First, smooth combustion profiles are studied where the combustion is modeled using the Vibe function, and parametric optimization is used to search for the optimal profile. Then, the most efficient combustion process with a completely free combustion is studied with theory and software for optimal control. A parameter study is performed to analyze the impact of crevice volume and air/fuel ratio λ . The results show that the losses have a high impact on the behavior, which is natural, and that the crevice effect has a very distinct effect on the optimal combustion giving a two mode appearance similar to the Seiliger cycle.

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1. INTRODUCTION

With the drive and strive for efficient combustion engines several things are investigated. One thing that has received much attention is the optimal placement of the combustion in relation to the crank angle revolution, and where 50% mass fraction burned has been used in rule of thumbs. Here the investigation will be taken one step further by looking at the complete combustion trace and asking the question what is the most efficient combustion trace. This is partly motivated by the availability to advanced fuel injection systems where the rate of fuel injection can be controlled which could allow rate shaping of the combustion. The other motivation is the fundamental question about how the optimal profile looks like if it could be selected freely. Rate shaping of the combustion is an interesting option for optimizing the performance of combustion engines, and the question studied here is how one can find the optimal heat release rates and how they vary for varying conditions.

To find the optimum heat release profile a methodology is developed that uses available theory and methods that allows us to use state of art optimal control software to solve the optimum combustion trace for a model. The method developed focuses on the combustion rate for optimal fuel economy, but the method is general as it can also be used for emissions provided that there is a model available.

Focusing on the torque and fuel economy it is well known know that a single zone model is sufficient for describing the engine cylinder pressure and thereby the amount of work produced and therefore the engine efficiency. The model uses the components in the well known

Gatowski et al.-model [1]. Experimental data are used to tune and validate the model, in order to get a representative model with good agreement to real engines.

According to theory with idealized cycles the instantaneous burning Otto cycle is the most efficient, however this is not true when considering losses such as heat transfer, and the impact of the losses are studied with the aid of the model.

The main contributions are:

- Modification of the Gatowski et al. model [1] that maintains simplicity within the framework of an ideal gas.
- A methodology for computing optimal burning trajectories, demonstrating that current optimal control software it is feasible to use for this application.
- New knowledge about optimum burn profiles for a variety of operating conditions.

The contributions are thus both the methodology and the resulting profiles themselves.

2. SINGLE ZONE MODELING

The reduction of the effects of heat transfer and mass loss on the cylinder pressure is called "heat release analysis" and is done within the framework of the first law of thermodynamics. The data reduction

also allows a consistency check of the pressure data itself. This model family can also be inverted to take a heat release trace and deliver a pressure as output.

A one-zone model offers the benefit of including heat transfer and gas flow in a simple manner. The combustion process is considered as a separate heat addition process and the contents of the chamber are regarded as a single fluid. Straightforward heat transfer and crevice models can then be used to complete the energy balance.

This paper makes some small extensions the well known model presented in the paper [1] by Gatowski et al. that develops, tests and applies a heat release analysis procedure that maintains simplicity while including the effects of heat transfer and crevice flows. The heat release model is a one zone description of the cylinder contents. The thermodynamic properties are represented by a linear approximation for $\gamma(T)$. The cylinder pressure is influenced by combustion, volume changes, heat transfer to the chamber walls, and mass leakage.

3. THE BASIC MODEL

The analysis and the model relies on the the first thermodynamic law that states

$$dU = \delta Q_{ch} - \delta Q_{ht} - \delta W - \sum_{i=1}^n dm_i h_i$$

where the directions of the heat, work, and enthalpy flows are defined according to Figure 1.

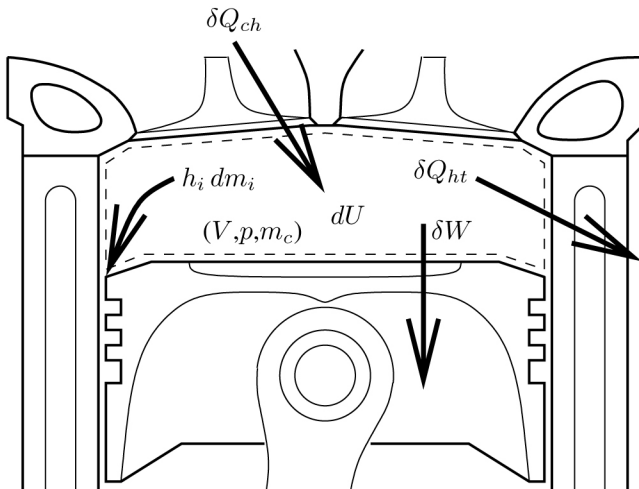


Figure 1. Thermodynamic control volume analysis for the combustion chamber, defining the directions of positive flows. The state is specified by (V, p, m_c) .

During the combustion, chemical energy is transformed into thermal energy of the charge through a change in composition from the unburned mixture to burnt reaction products. Standard thermodynamics represents this by considering the internal energy of the unburned mixture as the sum of a heat of formation at reference conditions and a sensible energy difference. The internal energies of both products and reactants are referred to the same datum so one can

determine the adiabatic flame temperature. However in single zone models the working fluid is considered to be homogeneous and the heat that is released from the combustion is considered to heat up the cylinder contents so the released heat from the chemical reactions is represented by δQ_{ch} in the equations above and this raises the internal energy of the cylinder contents. The computation of the single zone heat release is expressed as follows

$$\delta Q_{ch} = dU_s + \delta W + \delta Q_{ht} + \sum_{i=1}^n h_i dm_i$$

where the positive flow direction is out of the combustion chamber. The work is piston work which is equal to

$$\delta W = p dV$$

If it is assumed that there is only one flow the mass in the cylinder m_c will decrease with the same rate as the out-flow $dm_c = dm_p$, giving

$$\delta Q_{ch} = dU_s + p dV + \delta Q_{ht} - h' dm_c$$

Where h' is the specific enthalpy of the flowing fluid, that depends on the flow direction. The change in sensible internal energy is calculated by assuming it as a function of the mean charge temperature only, $U_s = m_c u(T)$, which is the ideal gas assumption

$$dU_s = m_c c_v(T) dT + u(T) dm_c$$

here m_c is the charge mass, and c_v is the mass average specific heat at constant volume. The mean temperature is determined by the ideal gas law,

$$T = \frac{pV}{m_c R} \quad (1)$$

Although this technique for calculating dU is not exact, the mean temperature found from the ideal gas law is close to the mass averaged cylinder temperature since the molecular weights of the reactants and products are nearly identical [1].

Inserting the internal energy differential into the energy equation gives

$$\delta Q_{ch} = m_c c_v(T) dT + p dV + \delta Q_{ht} + (u(T) - h') dm_c$$

In the next step a further simplification of the expression is performed, in particular dT is expressed as a function of dV , dp and dm , which is achieved by using the ideal gas law in both its normal form and differential form.

$$m_c R dT + T R dm_c = p dV + V dp$$

(here again the assumption of an ideal gas is used, which means that the change in the gas constant is neglected) rearranging the terms and multiplying with c_v gives

$$m_c c_v dT = \frac{c_v}{R} p dV + \frac{c_v}{R} V dp - c_v T dm_c$$

Another component to rewrite is the enthalpy h' where the ideal gas law $p'v' = RT'$ is used together with the definition $h(T') = u(T') + p'v' = u(T') + RT'$. Finally all is put together with the temperature dependence included explicitly in the energy and specific heats

$$\delta Q_{ch} = \frac{c_v(T)}{R} V dp + \frac{(c_v(T) + R)}{R} p dV + \delta Q_{ht} + (u(T) - (u(T') + RT') - c_v(T) T) dm_c \quad (2)$$

in the original paper [1] c_v , R , and $u' - u$ were expressed using a model for $\gamma(T)$, but here the manipulations are stopped since new models for $c_v(T)$ and $u(T)$ can be used directly in (2). These will be developed in the next step. Thereafter, the model for the combustion chamber flow dm_c , which is into and out of crevices, will be studied.

Modification 1: New Gas Property Model

The sensitivity analysis performed on the model in [2] shows that the model for the gas properties γ is the most important parameter in the Gatowski et al. model. This motivated the study and search for an alternative model for γ in [2]. Further publications that highlights the importance of the gas properties are [3, 4], whereof the first presents a high polynomial degree model for c_v and the latter modifies the Gatowski approach. With these previous approaches it is still difficult to include the crevice effect and maintain simplicity in the equations, as commented on in [2].

Here the goal is to improve the property model while giving a simple calculation scheme for the both the analysis procedure and the crevice model. This is achieved by staying with an ideal gas model and exchanging the linear $\gamma(T)$ model with a higher order polynomial model for the internal energy $u(\lambda, T)$ and $c_v(\lambda, T)$. Looking at thermodynamic data for γ one sees that the air to fuel ratio shifts the properties. In [5] it was implemented so that the offset of gamma was allowed to shift. This shift is incorporated directly in the method here where λ is included as a parameter in the property models.

In a single zone model the absolute level of the energy is not needed as the process mainly deals with changes and differences in properties. With a two zone model the absolute value would be needed to determine the combusted gas temperature, so there is also a component for this in the model here.

For lean conditions $\lambda > 1$ and at high pressures where there is little dissociation and the internal energy and specific heat can be captured well with the following structure of the polynomial in temperature and mixture strength

$$u_s(\lambda, \tilde{T}) = l_1 \lambda \tilde{T} + l_2 \lambda \tilde{T}^2 + l_3 \lambda^2 \tilde{T}^2 + c_1 \tilde{T} + c_2 \tilde{T}^2 + c_3 \tilde{T}^3 + c_4 \tilde{T}^4 + c_5 \tilde{T}^5 \quad (3)$$

where $\tilde{T} = \frac{T-300}{1000}$, with T given in K. This gives an internal energy that function that is identical to 0 at $T=300$ K, differentiating this gives

$$c_v(\lambda, \tilde{T}) = \frac{1}{1000} (l_1 \lambda + 2 l_2 \lambda \tilde{T} + 2 l_3 \lambda^2 \tilde{T} + c_1 + 2 c_2 \tilde{T} + 3 c_3 \tilde{T}^2 + 4 c_4 \tilde{T}^3 + 5 c_5 \tilde{T}^4) \quad (4)$$

The model is tuned to burned gas equilibrium data, obtained from the CHEPP [6]. For completeness the absolute internal energy is modeled as second order polynomial in λ

$$u_{300}(\lambda) = u_0 + u_1 \lambda + u_2 \lambda^2$$

so the full function for the internal energy becomes is

$u(\lambda, T) = u_{300}(\lambda) + u_s(\lambda, \tilde{T}(T))$ The resulting model parameters are given below and the fit to equilibrium data is shown in Figure 2. The absolute internal energy at $T = 300$ K is shown below in Figure 3.

$$\begin{array}{l} c_1 = +8.26159 \cdot 10^5 \\ c_2 = +1.65422 \cdot 10^5 \\ c_3 = +1.02150 \cdot 10^5 \\ c_4 = -0.85770 \cdot 10^5 \\ c_5 = +0.21236 \cdot 10^5 \end{array} \quad \begin{array}{l} l_1 = -0.39486 \cdot 10^5 \\ l_2 = -0.90978 \cdot 10^5 \\ l_3 = +0.26322 \cdot 10^5 \end{array} \quad \begin{array}{l} u_0 = -6.20236 \cdot 10^6 \\ u_1 = +4.13857 \cdot 10^6 \\ u_2 = -0.91531 \cdot 10^6 \end{array}$$

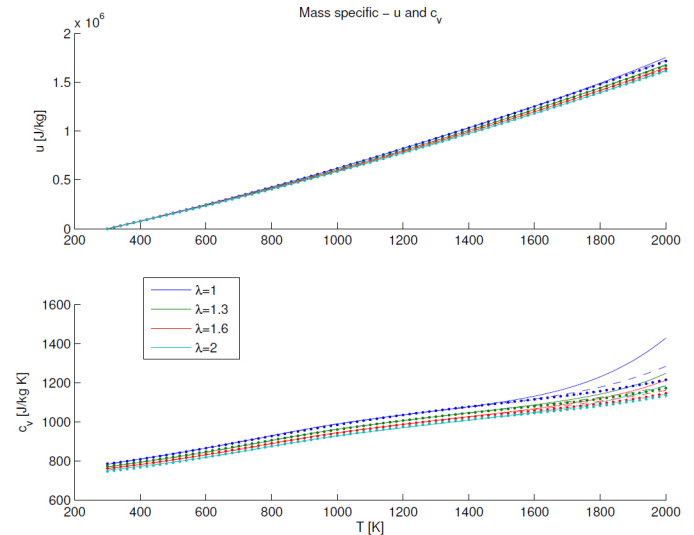


Figure 2. Model and its validation for the temperature range 300-2000 K, (solid lines $p=1$ atm, dashed $p=10$ atm, dotted $p=100$ atm). At high temperatures $T > 1400$ K and low pressures, there is dissociation but this is neglected in the model. The model has thick dots, while the non dissociation data has thin dots.

Furthermore for lean conditions molecular weight is also almost constant, with $M \approx 0.0286$ kg/mol giving $R \approx 290$ J/kg K.

Another modification is to allow the mass in the cylinder to vary and use the varying mass for temperature determination.

Crevice Effect

Crevice walls are cold and narrow and the volume is small so gases in the crevice is assumed to be close to the wall temperature. Due to these facts the crevices may contain substantial amounts of gas

during the period when the cylinder pressure is very high. Some gas blows by the top ring into the volumes behind the rings and some of this ends up in the crankcase.

A simple model which does not account for blowby is to consider a single aggregate crevice volume with the same temperature as the wall and the same pressure as the cylinder, i.e. $m_{cr} = \frac{pV_{cr}}{RT_w}$. In this model it is assumed that there is no blow-by past the piston rings so all mass stays in the combined volume of the cylinder and the crevice. See Figure 4 for a sketch of the situation, illustrating that the considered volume is above and behind the uppermost piston ring. In the model here the single mass flux term considered, is the flow of gas into and out of the crevice regions. The total trapped mass is divided into the cylinder mass and the crevice mass

$$m_{tot} = m_c + m_{cr} \quad (5)$$

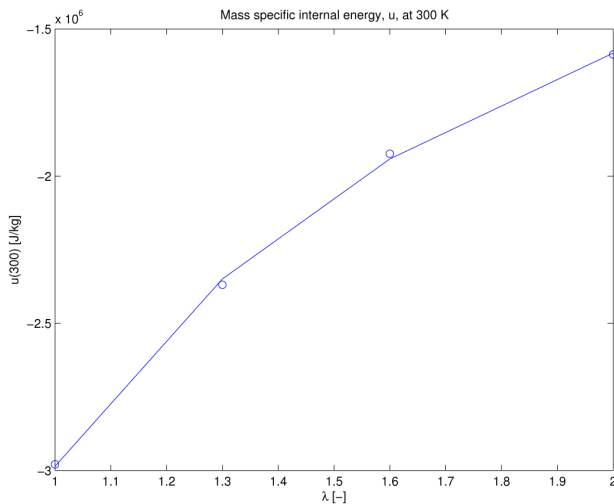


Figure 3. Model for the absolute internal energy at 300 K, as a function of λ . Solid - data, dots - Model. Data is generated by CHEPP [6].

Without blow-by, m_{tot} is constant which gives the following relation for mass transfers between crevice and cylinder

$$dm_c = -dm_{cr}$$

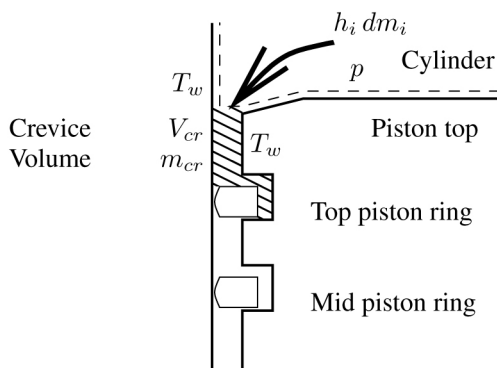


Figure 4. Sketch of the crevice model with the volume above and behind the top ring. The pressure in the crevice is the same as in the cylinder, while the gases that enter the crevices quickly become cooled and assume the same temperature as the wall temperature. The mass in the crevice is therefore determined from the ideal gas law with the aggregated crevice volume, cylinder pressure, and wall temperature.

This gives,

$$dm_c = -dm_{cr} = -\frac{dp V_{cr}}{R T_w}$$

which inserted into (2) gives

$$\begin{aligned} \delta Q_{ch} = & \frac{c_v}{R} V dp + \frac{(c_v + R)}{R} p dV + \delta Q_{ht} \\ & + dp \frac{V_{cr}}{R T_w} \left(u(T') - u(T) + R T' + c_v(T) T \right) \end{aligned} \quad (6)$$

Where

$$T' = \begin{cases} T & \text{if } dp > 0 \\ T_w & \text{if } dp < 0 \end{cases} \quad (7)$$

Here it is worth to note that it is the difference in internal energy that is evaluated and therefore only the sensible part is needed, $u(T') - u(T) = u_s(T') - u_s(T)$. The internal energy and specific heat depend on λ , and this dependence is omitted here in order to keep the nomenclature simple, this is done since λ is assumed to be constant throughout the cycle.

As a side note on the importance of the crevice. The percentage of the original charge present in the crevice at the end of the combustion can approach 10%.

Modification 2: Using Internal Energy Directly

In the original paper the linear model for $\gamma(T)$ was used to determine the internal energy difference, which resulted in a logarithm of a quotient. With the new property model it is possible to use the internal energy model (3) directly

Modification 3: Allowing a Variation in Mass for the Temperature Calculation

In the original model [1] the cylinder gas temperature is determined from the ideal gas law (1) but it is not explicitly stated how m_c is calculated there, so many implementations use the following expression

$$T = T_{ivc} \frac{p V}{p_{ivc} V_{ivc}}$$

Which only requires inlet valve closing conditions to be known and does not need m_c or R . However this model corresponds to the assumption that the cylinder mass is constant during the cycle. Here the total mass (5) is considered constant which is determined at intake valve closing to

$$m_{tot} = \frac{p_{ivc} V_{ivc}}{R T_{ivc}} + \frac{p_{ivc} V_{cr}}{R T_w}$$

For every p and V the cylinder mass can now be calculated