

Calculation of Optimal Heat Release Rates under Constrained Conditions

Lars Eriksson and Martin Sivertsson
Linköping University

ABSTRACT

The work extends a methodology, for searching for optimal heat release profiles, by adding complex constraints on states. To find the optimum heat release profile a methodology, that uses available theory and methods, was developed that enables the use of state of the art optimal control software to find the optimum combustion trace for a model. The methodology is here extended to include constraints and the method is then applied to study how sensitive the solution is to different effects such as heat transfer, crevice flow, maximum rate of pressure rise, maximum pressure, knock and NO generation. The Gatowski single zone model is extended to a pseudo two zone model, to get an unburned zone that is used to describe the knocking and a burned zone for NO generation. A modification of the extended Zeldovich mechanism that makes it continuously differentiable, is used for NO generation. Previous results showed that the crevice effect had a significant influence on the shape for the unconstrained case where a two mode combustion was seen, one initial pressure rise and one constant pressure phase. Here it is shown that it still has a significant influence on the appearance until the maximum pressure limit is reached and becomes the dominating constraint. In the unconstrained case no conditions had combustion before TDC all started after, but when limitations are considered and come into play the combustion can now start before TDC to avoid excessive losses during the expansion. When introducing constraints on the NO formation through the extended Zeldovich mechanism the combustion takes the shape of a three mode combustion, one initial rapid burning, one later rapid burning and a constant pressure phase. In summary it is shown that the methodology is able to cope with the introduced constraints.

CITATION: Eriksson, L. and Sivertsson, M., "Calculation of Optimal Heat Release Rates under Constrained Conditions," *SAE Int. J. Engines* 9(2):2016, doi:10.4271/2016-01-0812.

1. INTRODUCTION

There is a continuous effort to develop efficient combustion engines and 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 to find the optimal placement. Looking at it in a more generalized sense, it becomes a question of optimal control where one can ask what the optimal combustion looks like. The first papers that connect optimal control to combustion are [1] where the optimal piston motion is derived to a model with friction losses and heat transfer, and [2] where constraints on acceleration, deceleration, and cycle time have also been considered. In recent papers [3, 4] the investigations assume that the crank mechanism is fixed and they study the complete combustion trace, asking the question: What is the most efficient shape of the 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 is how one can find the optimal heat release rates and how they change with 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 here extends the work in [3], with the addition of constraints such as maximum pressure and pressure rise rates, as well as knocking and also NO emissions.

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 [5] that was extended in [3]. In the extension here special emphasis has been on a model that are two times continuously differentiable (called C^2 functions) so that gradients and Hessians can be calculated by Automatic Differentiation (AD) software during the search for the best burn profiles.

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 crevice effects and especially when also adding constraints on combustion and emissions.

The main contributions of the paper are:

- The development of a model and optimal control methodology that can include several dynamic states (here 4 states plus an integral state for the criterion) without the curse of dimensions present in dynamic programming.
- Study of the combined effects of heat transfer, crevice effect, and limitations on pressure rise rate, maximum pressure, knock, and NO generation.
- The mathematical formulation of the extended Zeldovich mechanism for NO belonging to the C^2 class so that it can be analytically differentiated by an AD tool and used efficiently by an optimal control software.
- New knowledge about optimum burn profiles and how the limiting factors influence the optimal burn rates.

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

2. THE SINGLE ZONE SIMULATION MODEL

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 is based on the model in [3] that makes an extension of the well known model by Gatowski et al., presented in the paper [5] 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. All model equations from [5] and with the extensions from [3] are included in the [Appendix](#) of this paper for completeness as many of the results depend strongly on the model details. The model is also extended in [Section 3](#) to a semi two-zone model that approximately tracks the burned and unburned gas temperatures.

Central Model Equations

The model is summarized below and details are given in [Appendix A](#). The analysis and the model relies on the the first thermodynamic law that states

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

where the directions of the heat, work, and enthalpy flows are defined according to [Figure 1](#). This model is manipulated and developed in the [appendix](#) which results in (25) that gives an expression for the pressure differential dp so we can calculate (i.e. simulate) the pressure.

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

This equation is expressed with differentials so that one can select either time t or crank angle θ as independent variable, selecting crank angle θ as independent variable and inserting the sub-models from the [appendix](#) gives the following model

$$h_c = \frac{0.013 p^{0.8} \left(C_1 u_p + \frac{C_2 (p-p_0) T_{lvc} V}{p_{lvc} V_{lvc}} \right)^{0.8}}{B^{0.2} T^{0.53}} \quad (2a)$$

$$\frac{\delta Q_{ht}}{d\theta} = \frac{A (T - T_w)}{\omega_e} h_c \quad (2b)$$

$$\frac{\delta Q_{ch}}{d\theta} = u \quad (2c)$$

$$\frac{dp}{d\theta} = \frac{dp_n}{dp_d} \quad (2d)$$

where u is the input heat release and where the following notation for the numerator and denominator is introduced

$$dp_n = \frac{\delta Q_{ch}}{d\theta} - \frac{\delta Q_{ht}}{d\theta} - \frac{(c_v(T) + R)}{R} p \frac{dV}{d\theta} \quad (3a)$$

$$dp_d = \frac{c_v(T)}{R} V + \frac{V_{cr}}{R T_w} \left(u(T') - u(T) + R T' + c_v(T) T \right) \quad (3b)$$

Note that in the expressions above the area A , volume V , and volume derivative $\frac{dV}{d\theta}$ are functions of the crank angle θ .

During the simulation the direction of the crevice flow needs to be determined, which depends on the sign of dp . See [Figure 13](#) in the [Appendix](#) for a sketch and the discussion around (23) and (24) for how the effects enter the equation. Noting that the denominator

dp_d is strictly positive enables us to only study the sign of the numerator dp_n to determine the flow direction and thus determine T' . Therefore the simulation is implemented so that the numerator is first calculated which determines the sign of dp and thus T' which in its turn is inserted into denominator and the full $\frac{dp}{d\theta}$ is calculated. The denominator in (2) changes depending on whether the flow is into or out from the crevice volume. This introduces a discontinuity into the model which destroys the desired C^2 property of the model. Therefore the function is smoothed out, using a tanh-function as follows:

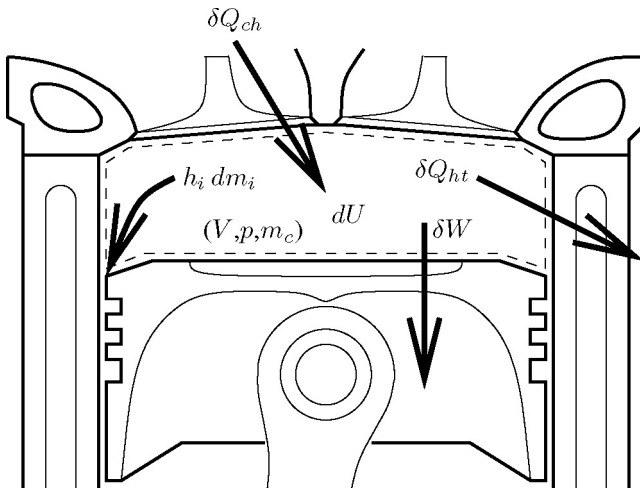


Figure 1. Thermodynamic control volume analysis for the combustion chamber, defining the directions of positive flows. The state is specified by (V, p, m_c) .

$$dp_d = dp_d(T_w) + \frac{1 + \tanh(10^4 dp_n)}{2} (dp_d(T) - dp_d(T_w)) \quad (4)$$

In the model we need the mean gas temperature and it is determined from the cylinder gas mass by the ideal gas law,

$$T = \frac{pV}{m_c R} \quad (5)$$

where the cylinder gas mass is the total mass minus the mass in the crevice, for more details see the discussion around (26) in the Appendix.

Specifying the Heat Release

In (2) the heat release $\frac{\delta Q_{ch}}{d\theta}$ is an input and this will be described differently in two cases. In the model validation, Section 4, where the combustion is considered smooth it will be prescribed with the well known Vibe function [6], see also Appendix A for details. In the model validation the Vibe parameters are adjusted so that the modeled pressure agrees with the measured. In the optimal control problem, Section 5, the heat release is selected freely by the optimizer under the constraint that it must be monotonously increasing.

3. EXTENSION TO A SEMI TWO-ZONE MODEL

The basic model is here extended with NO_x and knock models, and to achieve that it is necessary to track the unburned and burned temperatures. This is done by defining three phases, going between Intake Valve Closing (IVC), Start Of Combustion (SOC), End Of Combustion (EOC), and Exhaust Valve Opening (EVO).

- During phase 1, IVC-SOC, there is only one zone, the unburned zone.
- During phase 2, SOC-EOC, there is semi-two zone model burned+unburned. Where following three temperatures are tracked, cylinder average T from the Gatowski model, unburned gas temperature T_u , and burned gas T_b .
- During phase 3, EOC-EVO, there is only one zone, the burned.

In phases 1 and 3 there is only one temperature, the average. The unburned gas temperature T_u is the same as the single zone temperature T up to start of combustion, thereafter it is approximated by a polytropic compression and expansion

$$T_u(\theta) = T(\theta_{soc}) \left(\frac{p(\theta)}{p(\theta_{soc})} \right)^{\frac{k-1}{k}} \quad (6)$$

with polytropic exponent k . In phase 2 the average temperature is considered to be a mix of the burned and un-burned temperatures. Assuming that they have the same specific heats gives the following expression for the average temperature

$$T(\theta) = (1 - x_b(\theta)) T_u(\theta) + x_b T_b(\theta)$$

With the average temperature given by the single zone model (5), the equation above can now be solved for $T_b(\theta)$

$$T_b(\theta) = \frac{T(\theta) - T_u(\theta)}{x_b(\theta)} + T_u(\theta) \quad (7)$$

where we need to consider and handle the special case of $x_b(\theta_{soc}) = 0$ to avoid division by zero. Early after θ_{soc} while $x_b(\theta)$ is small this model can be sensitive to model errors in the unburned trace, for example if the polytropic exponent doesn't give a good representation of how the unburned gas behaves thermally when it is compressed. This might cause $T_b(\theta)$ to vary significantly. To fill in the gap near $x_b = 0$ the following supporting function is used

$$T_b(\theta_{soc}) = T_u(\theta_{soc}) + \Delta T_{ad} \quad (8)$$

where ΔT_{ad} is the temperature rise in an adiabatic flame [7, Figure 6.7]. Then a tanh weighting function is used to avoid problems when switching from the adiabatic flame temperature to that which is calculated from the adiabatic mixing in (7).

In the next step two submodels that utilize the two temperatures (6) and (8) will be discussed. The models are a knock model that is driven by the unburned temperature T_u and an NO model that is driven by the burned temperature T_b .

Knock Model

Knocking occurs in the unburned zone and the reactions that drives the gases towards knock are influenced by the unburned temperature. Here the simple knock integral model, [8, 9], is used

$$KI(\theta) = \int_{\theta_{ivc}}^{\theta} \frac{1}{\tau(ON, T_u(\alpha), p(\alpha))} d\alpha$$

where the ignition delay $\tau(\cdot)$ is modeled using the Arrhenius function that comes from [10] (with parameters adapted to SI engines according to [8, p. 468])

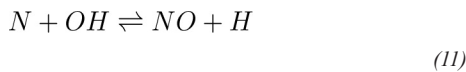
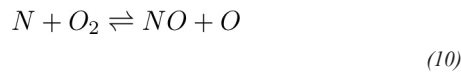
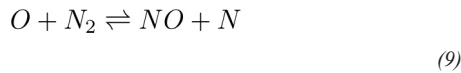
$$\tau(ON, p, T_u) = 0.01768 \left(\frac{ON}{100} \right)^{3.402} p^{-1.7} e^{\frac{3800}{T_u}}$$

In this model, knock is said to occur at the angle when $KI(\theta)$ reaches a limit L , for example the knocking angle θ_{kn} is set to $KI(\theta_{kn}) = L$, often the model parameters are tuned so that $L = 1.0$ when running on experimental data. In some cases it is said that the engine is safe from knock as long as $KI < L$ for $x_b < 0.75$, [11], meaning that there is not sufficient mass left to give a damage when knock occur.

NO Model

NO is formed in the hot burned gases and the formation is driven by the burned gas temperature, and this is the motive for the extension of the single zone model to a pseudo two zone model.

Normally it is stated that the most dominant NO forming mechanism is the thermal formation which is frequently modeled using the extended Zeldovich mechanism [8].



originating from [12] with (11) added by [13]. This is a much studied system of reactions that is often simplified and rewritten to one single differential equation for the NO concentration (see [13])

$$\frac{d[NO]}{dt} = 2 R_1 \frac{1 - \left(\frac{[NO]}{[NO]_e} \right)^2}{1 + \frac{[NO]}{[NO]_e} \frac{R_1}{R_2 + R_3}} \quad (12)$$

where R_i are the equilibrium reaction rates defined by

$$R_1 = k_1^+ [O]_e [N_2]_e = k_1^- [NO]_e [N]_e \quad (13a)$$

$$R_2 = k_2^+ [N]_e [O_2]_e = k_2^- [NO]_e [O]_e \quad (13b)$$

$$R_3 = k_3^+ [N]_e [OH]_e = k_3^- [NO]_e [H]_e \quad (13c)$$

where $[\cdot]_e$ are equilibrium concentrations and were k_i^+ and k_i^- are the forward and reverse reaction rate constants of the three reactions (9),(10),(11). There is a strong temperature dependence in the formation rates k_i making it necessary to account for the temperature dynamics in the analysis of the formation. To calculate the R_i 's one normally uses an equilibrium program to calculate the equilibrium concentrations that is either used on the fly in the simulation or the values are pre-calculated and stored in look-up tables. In the implementation here a continuously differentiable function is developed to capture the behavior of the equilibrium so that the Algorithmic Differentiation (AD) software can differentiate the equations while searching for the optimal trajectories.

After studying the general behavior of equilibrium concentrations that range over several magnitudes and has a convergence towards zero, as function of temperature, that is faster than exponential the following equation for a general equilibrium concentration is proposed

$$y(T) = c_1 e^{-c_2 \left(\frac{T - c_3}{1000} \right)^{c_4}} \quad (14)$$

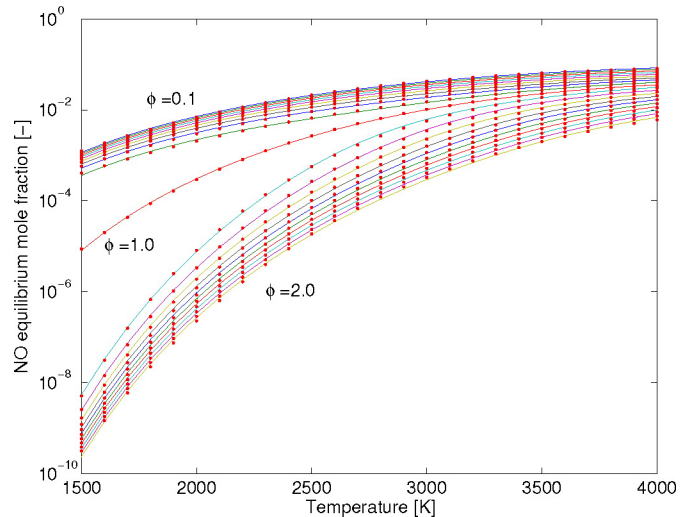


Figure 2. Equilibrium concentration for NO as function of temperature and λ high lambda gives higher NO concentrations. The single line between the lean and rich groups is $\lambda = 1$. The dots are the results from using (14).

c_1 to c_4 naturally varies with the molecule (for example NO) and the air/fuel ratio λ . The function is shown together with the equilibrium concentrations obtained by CHEPP [14] for NO in Figure 2. Note that the scale is logarithmic on the y-axis, if the convergence towards zero would be exponential it would appear as a line in the figure. From the figure it is seen that the concentrations go to zero faster than an exponential. This motivates functional expression with a power function in the exponent in (14).

There is also a significant dependence on λ . Here λ is considered fixed during the cycle and for the desired lambda the function (14) can be fitted to equilibrium data $[NO]_e$ and used in (12).

To get the complete Zeldovich mechanism there is a need to calculate the R_i 's in (13), that are also temperature dependent. Studying (12) one sees that one only needs to calculate $R_1(T_b)$ and the quotient

$$Q(T_b) = \frac{R_1(T_b)}{R_2(T_b) + R_3(T_b)}$$

The rate $R_1(T_b)$ varies over 30 magnitudes, see Figure 3, and also goes to zero faster than an exponential, here the same functional form (14) is used to model the rate. The quotient $Q(T_b)$ varies much less but has also a special behavior for $\lambda = 1$, to keep things simple it is also modeled with an exponential variation of (14).

To summarize the NO formation, we now define a composite function that is composed of the three other functions, $[NO]_e(T_b)$, $R_1(T_b)$, and $Q(T_b)$

$$f_{NO}([NO], T_b) = 2 R_1(T_b) \frac{1 - \left(\frac{[NO]}{[NO]_e(T_b)} \right)^2}{1 + \frac{[NO]}{[NO]_e(T_b)} Q(T_b)} \quad (15)$$

With the aid of this function the NO formation is now modeled with the following composite function

$$\frac{d[NO]}{dt} = c_{NO} f_{NO}([NO], T_b) \quad (16)$$

The model has a wide variation of the rates and equilibrium concentrations as seen in Figures 2 and 3 and it was sensitive to model tuning errors. Therefore, an additional gain c_{NO} was added to (16) that allows the function to be adjusted to fine-tune the NO generation.

The procedure applied here is that a λ is selected then an equilibrium program (e.g. NASA [15] or CHEPP [14]) is run to calculate $[NO]_e$ and all other concentrations that are needed in (13) to determine R_1 and Q , then three versions of (14) are fitted to the data giving one parameter set of c_1 to c_4 for each of the three functions $[NO]_e(T_b)$,

$R_1(T_b)$, and $Q(T_b)$. All in all providing the composite function (15) which gives a differentiable function $f_{NO}([NO], T_b)$ which can be used in an optimal control software that relies upon AD software giving efficient search methods.

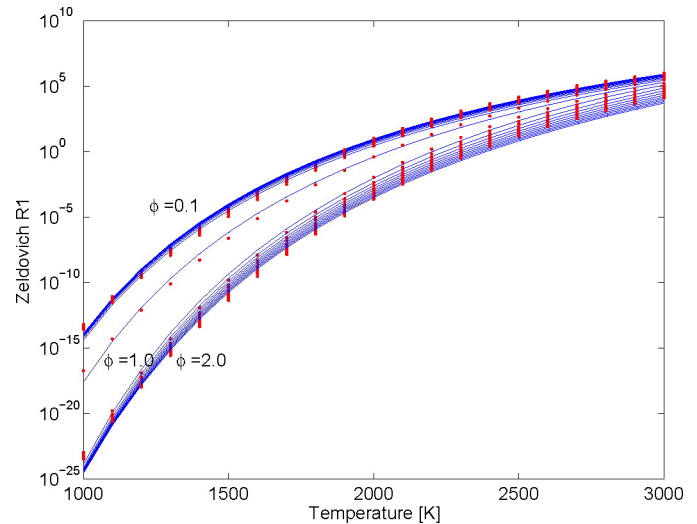


Figure 3. Rate R_1 in the Extended Zeldovich model.

The function for NO generation (16) is finally fine-tuned so that it agrees with the rates calculated using the results from an equilibrium program. The tuning is performed so that the freezing effect in NO is seen and that the NO concentrations become reasonable, see Figure 5. If c_{NO} is too high the concentration will follow the equilibrium and if it is too small too little NO will be generated.

4. QUANTITATIVE AND QUALITATIVE MODEL VALIDATION

The nominal operating point is selected to be in the mid operating region where the engine frequently operates during normal driving, i.e. this is a point of importance for fuel economy of the engine, and it was used in the original paper. This nominal operation point is therefore kept so that the results can be related to those of the original paper. The point is far away from critical conditions like knocking and other limits coupled to engine design and operation such as maximum pressures and temperatures, so these will be introduced more artificially to show that the optimization can handle general constraints.

The parameter tuning method and default parameters are described in detail in [3]. Figure 4 shows is a quantitative validation of the single zone model for a normal cycle, where it is seen that the agreement between the modeled and measured pressures is very good, the relative error in a single sample only about 1%, and for the work production over the interval the relative error is 1.2%. Showing that the model can describe the work production process in the cylinder very accurately.

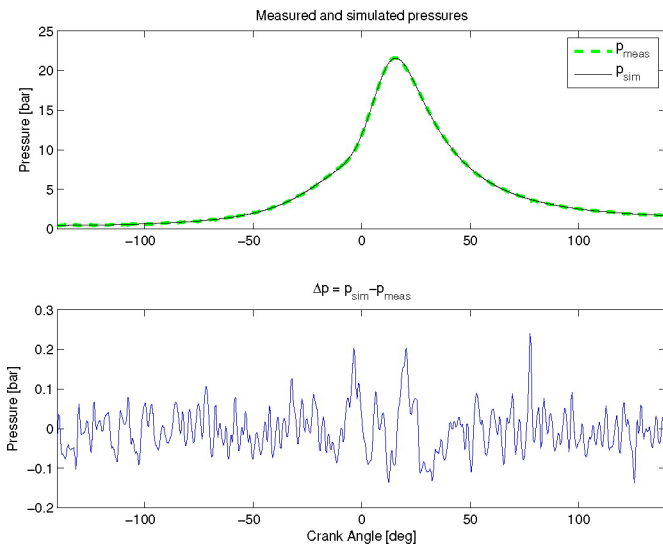


Figure 4. Quantitative model validation of the implemented model. Top: Measured and simulated pressure. Bottom: Difference. A maximum error of 0.2 bar and maximum pressure of 20 bar gives a relative error of 1%. The difference in work output between the model and measurement 0.28 J, while the total work is 233.0 J which is 1.2%.

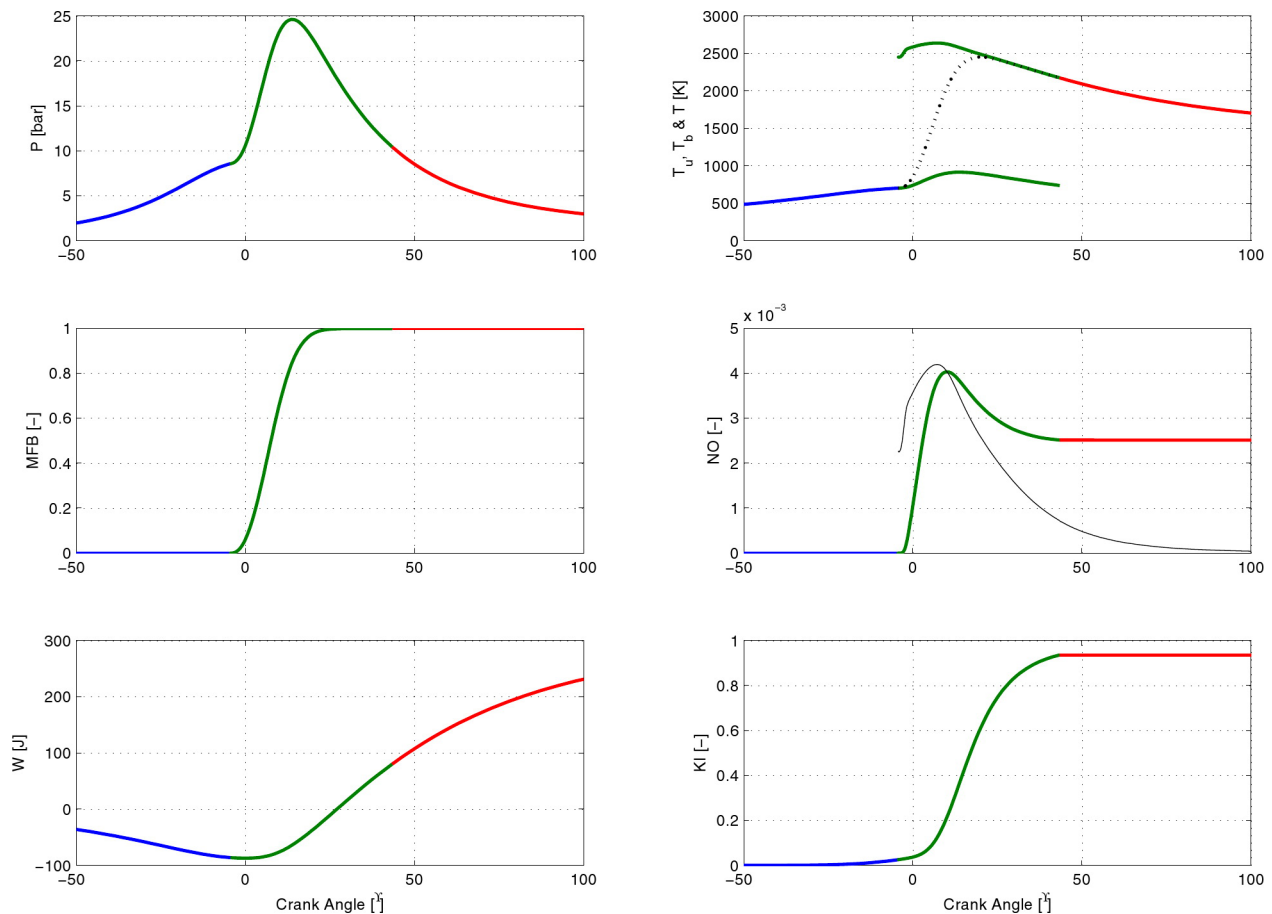


Figure 5. Qualitative model validation of the implemented model. The plots show the three phases (1-blue, 2-green, 3-red) for the simulated signals: pressure, mass fraction burned, cumulative produced work, temperatures (unburned, average and burned), NO production and knock index. In the NO-plot there is a thinner black line that is the equilibrium concentration. The qualitative behavior agrees with that one can find in the combustion engine literature.

The extended model, with extensions to knocking and NO production, is only validated qualitatively. The fuel optimal burn profile computed using the smooth combustion specified with the Vibe function in [3] is selected as the nominal case. The resulting cylinder pressures, temperatures, knock index, NO generation, and work for the new extended model is shown in Figure 5. This is then compared to profiles in the standard literature, showing that the resulting profiles agrees with what is expected, for example NO equilibrium and freezing phenomenon has the familiar shape as is shown in [8, Figure 11-7].

5. OPTIMAL CONTROL PROBLEM FORMULATION

The model is valid from IVC to EVO so the optimal control problem is solved for that region, where a symmetric crank interval approximating IVC and EVO, is selected in the investigation below. The optimal control problem is formulated as follows: The produced work is to be maximized

$$\max W = \int_{-150}^{150} p(\theta, u) \frac{dV(\theta)}{d\theta} d\theta$$