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HEAT-RELEASE SHAPING FOR OPTIMAL REACTIVITY CONTROLLED COMPRESSION IGNITION

Anders Brink[a*], Paulo S.P. da Silva[a],Aneesh Vasudev[b], Maciej Mikulski[b], Jeudi Aro[c], Jari Hyvönen[c]
[a] *Åbo Akademi University, Turku, Finland*
[b] *University of Vaasa, Vaasa, Finland*
[c] *Wärtsilä Finland Oy, Vaasa, Finland*

ABSTRACT

A surrogate-based optimization routine is coupled with a Multi-Zone Model (MZM) for optimizing the combustion efficiency of a Reactivity Controlled Compression Ignition engine. In the first step, some model parameters are calibrated against experimental data. In the second step, initial reactive fuel distribution is determined by optimizing the engine's combustion efficiency. The results suggest that a highly stratified initial fuel distribution should be aimed for to maximize combustion efficiency.

Keywords: RCCI, optimization, fuel distribution

1. INTRODUCTION

Global shipping is responsible for approximately 3 % of worldwide greenhouse gas (GHG) emissions [1]. The shipping industry has set a target to reduce CO_2 emissions per transport work by at least 40% by 2030 and to reduce the annual GHG by at least 50% by 2050.

Today most ocean liners used diesel. Liquefied Natural Gas (LNG) is seen as an important transitional fuel. In addition to reducing CO_2-emission, the use of LNG also cuts other emissions, the most obvious one being SO_X. Natural gas engines are either typically lean-burn spark-ignited or dual fuel concepts. Using a lean-burn concept is a way to reduce NOx emissions and increase efficiency. The drawback of this concept is controllability and risk of misfire. Reactivity Controlled Compression Ignition (RCCI) is a dual-fuel concept, where compression ignition is achieved using a reactive fuel like diesel. The reactive fuel should be injected such that the formed mixture burns with high efficiency, avoiding too high pressure rise rates and too high maximum cylinder pressure. The process forming the distribution of the reactive fuel is complex and depends on a large number of parameters such as the start of injection, the duration of the injection, the injection pressure, and the injector itself. A large number of free variables makes the development experimentally challenging and expensive.

One alternative is to use a simulator coupled with an optimization routine [2]. To overcome computational problems surrogate model can be used. The surrogate model is constructed based on a limited number of function evaluations and a computationally cheap function fitted to the function output. Surrogate function based optimization has also been used in engine optimization, e.g., Navid *et al*. [3] compared two optimization algorithms using a surrogate function constructed from evaluations of a CFD model to find an optimal engine design.

While CFD modeling allows for detailed investigation of geometry design, this is still an extremely computationally demanding approach. Especially, for reacting flows it calls for simplifications and compromises. Reactor networks are an established method used to simplify fluid dynamics allowing one to focus on the chemistry. Pioneering work is that of Bragg [4], who modelled a flame as a perfectly stirred reactor followed by a plug flow reactor. In the combustion engine area reactor network models often goes by the name multi-zone model. Another pioneering work is that of Noda and Foster [5] who modeled Homogeneous Charge Compression Ignition (HCCI) with H_2 as a fuel. HCCI is a low temperature combustion concept similar to RCCI but does not involve fuel stratification. The authors divided the cylinder into zones based on assumed initial conditions and not based on their spatial location. In their study, they assumed a correlation between the initial fuel/air ratio and temperature. More recently, Aceves *et al*. [6] used a multi-zone model to study HCCI. The results from CFD calculations were used

*Corresponding author email: anders.brink@abo.fi

to divide the cylinder volume into zones. The authors also used results from the CFD simulations to assign a temperature history for each of the zones. In their model, all zones shred the same pressure, but apart from this, there was no communication between the zones. They found that for HCCI they could predict the maximum pressure, burn duration, and efficiency within 10%. Rakopoulos *et al*. [7] used a multi-zone model to study combustion in a direct-injection diesel engine. They used a two-dimensional zone model where droplet evaporation and jet mixing models were used to determine the amount of fuel and entrained air in each zone. Their model is characterized by a detailed model of the fuel spray, whereas the combustion chemistry is modeled using in a simplified way. A comprehensive review of multi-zone models is given by Vasudev *et al*. [8].

2. METHODS

2.1 Multi-Zone Model

The simulation of the natural–gas–light fuel oil RCCI is performed with the University of Vaasa Advanced Thermo-kinetic multi-zone. A detailed description of the testing and development of this model can be found in Vasudev *et al*. [9]. The model is implemented in C++ and utilizes libraries from Cantera [10]. The cylinder volume is divided into 12 zones. Figure 1 shows the zone distribution at the start of the calculations. The zones are plotted according to their relative volumes, so the location of the zone boundaries do not coincide with their radial positions due to the cylindrical geometry. As the zones share a common pressure whereas the temperature of the zones is modeled individually, the fraction occupied by a zone varies during the cycle. One zone is used as a boundary layer at the cylinder head, one at the piston and one zone are in contact with the liner. The two boundary layer zones are not numbered in the figure.

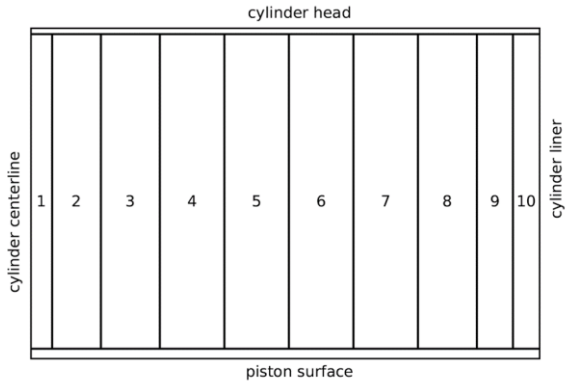

Figure 1. Initial zone distribution in the Multi-Zone model. The model assumes a cylindrical geometry, so the cylinder center centerline is the symmetry axis.

The zones exchange heat and mass with their immediate neighbors via turbulence based gradient driven transport. The approach is based on the work of Yang and Martin [11], with one calibrating constant to tune the model. A chemical mechanism for n-dodecane [12] is used to describe the combustion chemistry. In the simulations the diesel fuel is modelled as a single component (n-dodecane). The model is run for the part of the cycle when all valves are closed, i.e., excluding gas exchange. In addition, the injection of the reactive light fuel oil is not modeled in detail; instead, initial fuel distribution is set as calibration/optimization parameter.

2.2 Surrogate model-based optimization framework

A single run of the Multi-zone model requires approximately three minutes of CPU time on a PC. This makes the direct use of gradient-based methods on the model computationally expensive. To overcome this a surrogate model-based optimization routine is used. The implementation follows largely that of Regis and Shoemaker [13]. The surrogate model is built using radial basis functions, i.e., the function value depends on the distance from a point. To obtain the function values necessary for constructing the surrogate model the multi-zone model needs to be evaluated. This true function is typically referred to as a black-box function, as its mathematical form typically is unknown. Once the black-box function values are available, constructing the surrogate model only requires solving a linear regression problem. Hence, evaluating the surrogate model is computationally cheap. Surrogate models for non-linear constraints, depending on the multi-zone model output, are constructed in an identical way. All independent variables have a lower and an upper bound, i.e. they are said to be box-constrained. To initialize the surrogate models an initial set of points is used. In this approach, the points are selected based on a uniform random distribution.

The constrained optimization imposes some additional challenges. The algorithm relies on having an incumbent, i.e., the best solution that does not break the constraint. This can be challenging to find, and it may be possible that a separate optimization step is needed at the start to find such a point.

Although the surrogate model is constructed using linear regression, the radial basis functions are non-linear, giving rise to a constrained global optimization problem. The global optimization problem defined by the surrogate models could be solved with any method suitable for non-convex global optimization. However, as the surrogate model is only a representation accurate in the point previously evaluated, the candidate point is selected from a set of possible candidate points that are given a merit value based on both exploration and exploitation. Exploration means that points far from previously evaluated points are given a bonus and exploitation that points that have a good objective function according to the surrogate model is given a bonus. To include both modes the weight between exploration and exploitation is allowed to vary.

Once a candidate point has been evaluated using the black-box function, the surrogate model is updated and a new candidate point is determined. The optimization routine will theoretically find the optimal point, but in practice, the optimization is either run until no further

improvement is obtained or a pre-set maximum number of black-box function evaluations are reached. In this study, a multi-start strategy was used, which is a standard method for avoiding local minima.

2.3 Scope and procedures

The surrogate model-based optimization routine is used in two ways in this study. First, an optimization problem is solved for tuning the model to match experimental data. In this stage the optimization problem is to match the pressure-crank angle data as close as possible with the constraint that the cumulative heat release is within a given tolerance. Only four variables are tuned in this study, one is the initial temperature of the charge and one is the parameter in the model describing the turbulence/inter-zonal mixing. Two parameters are used to describe the initial distribution of the light fuel oil. This is done using a beta-function

$$B(a,b) = \int_0^1 x^{a-1}(1-x)^{b-1}dx.$$

The beta function is also used in pdf-based combustion models in CFD because of its great flexibility to adapt.

In the second stage, the surrogate model-based optimization is used to find a fuel distribution that maximizes the efficiency of during the closed-cycle period. At this stage only the two parameters describing the beta function are varied. The initial temperature and the values of the mixing parameter found during the tuning stage are maintained. The reasoning is that as only the fuel distribution is modified, these should not be affected.

3. RESULTS AND DISCUSSION

Figures 2a and 2b shows the initial fuel distribution in the case tuned to experimental data for a 50% load case.

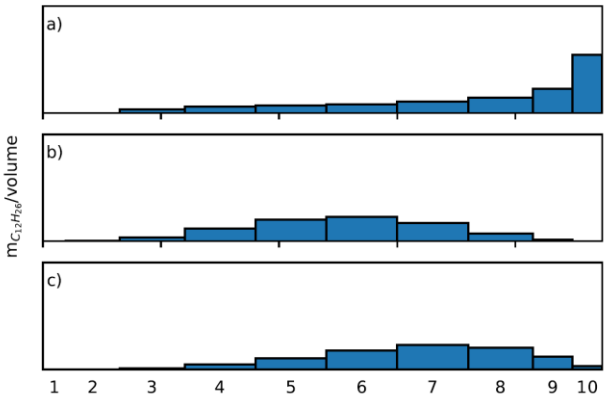

Figure 2. a) Dodecane distribution obtained using manual tuning to fit the experimental pressure trace. b) Dodecane distribution obtained tuning using a surrogate based global optimization routine. c) Dodecane distribution obtained when maximizing the combustion efficiency. The numbers below the figure give the zone numbers.

In Fig 2a the fuel distribution has been tuned manually according to a presumed reactive fuel distribution whereas in Fig 2b the distribution has been tuned using the optimization routine. The figure shows normalized mass of n-dodecane per volume. The volume will change during compression changing the absolute values, while the normalized values remains relatively unchanged until ignition occurs. Both cases where closely tuned to the experimental data, despite the difference in initial fuel distribution. Figure 2c shows the optimized fuel distribution. The work performed during the combustion stroke increases by 4.3 %, i.e., a relatively large improvement. The obtained optimal reactive fuel distribution differs strongly from the one tuned manually. One should remember that although the zones in the present model has a spatial locations, other MZM models choose to see the zones as representative conditions. In this model too, zones away from the cylinder wall experience similar heat transfer conditions. It is thus likely that its location could probably be shifted as long as the reactive fuel is highly stratified and has an s-shape.

Figure 3 shows the temperature evolution of the zones in the MZM in the three cases as a function of crank angle. The temperature evolution in the zones are different in the manually tuned case and the one tuned by optimization. The turquoise line represents the zone adjacent to the cylinder liner. In the manually tuned case, this is the first zone to ignite, whereas in the case tuned using the optimization routine this zone does not ignite. The case optimized for efficiency shows a more homogenous onset of the combustion in the whole cylinder. The two cold zones in the figure are those used to describe the boundary layers.

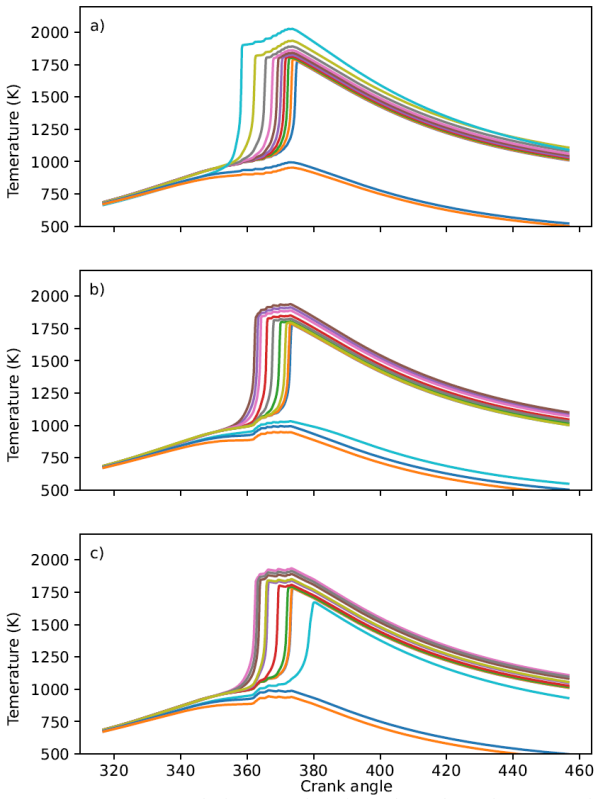

Figure 3. Temperature evolution as a function of crank angle. a) Result obtained using manual tuning to fit the experimental pressure trace. b) Result obtained tuning using a surrogate based global optimization routine. c) Result obtained maximizing the combustion efficiency.

Analyzing the solution in detail reveals that the air to fuel ratio, calculated using only n-dodecane and excluding the premixed natural gas present, is very high. The zones ignite according to the concentration of n-dodecane in the zones.

Figure 4 shows the net cumulative heat release (normalized) for the three different fuel distributions. The onset of ignition in a zone can be seen in the cumulative heat release curve. This is clearest in the manually tuned case, where the ignition the zones is more separated.

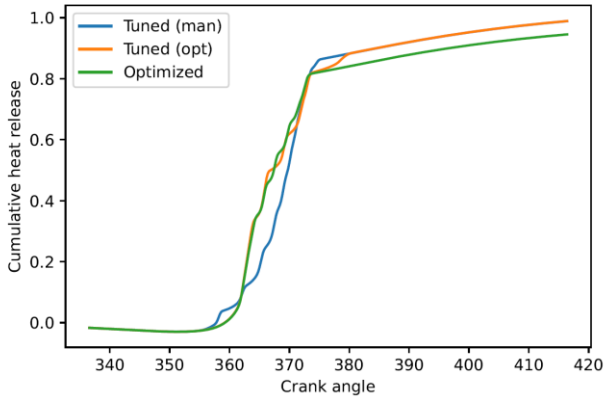

Figure 4. Net cumulative heat release (normalized) as a function of crank angle.

The figure reveals that in the manually tuned case the much of the heat release occurs late in the cycle, whereas in the case tuned using the surrogate based optimization routine the combustion is incomplete. This could also be deduced from Fig 3, where the zone next to the cylinder liner remained cold with this fuel distribution. With the fuel distribution optimized for efficiency, the heat release occurs around the top dead center (crank angle of 360°) while the combustion is more complete.

Finding the optimal initial fuel distribution does not solve the problem for an engine manufacturer as its formation depends on a large number of parameters. However, knowing the kind of fuel distribution to aim at still is highly beneficial in the design process.

4. CONCLUSIONS

This study demonstrates that a surrogate based optimization routine can been coupled with a Multi-zone model for optimizing RCCI combustion.

The results show that a significant improvement in efficiency can be achieved by optimizing the initial fuel distribution.

High efficiency is reached with a rapid combustion process allowing energy to be transferred to useful work shortly after the top dead center.

5. ACKNOLEDGEMENT

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