# AUTOMATIC OPTIMIZATION OF DETAILED KINETIC MECHANISM FOR HCCI-ENGINE SIMULATION

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## Introduction

In recent years detailed kinetic models have been developed and validated for both auto ignition and laminar combustion processes. The range of validity of these models is limited by the range of physical parameters covered by the available experimental data. At high pressure, for example, shock tube data for the validation of ignition delay times are available for the investigated fuels with air-fuel equivalence ratios smaller than 2.0. Homogeneous Charge Compression Ignition (HCCI) engines are known to be operated with fuel-air equivalence ratios greater than 2.0, or with high rates of Exhaust Gas Recirculation (EGR). These conditions are not within the range of validity of the available kinetic models, and a re-optimization of the models is necessary.

## Optimization

The optimization of reaction models has been automated in the past. The development of the GRI-Mech has been done using a semi-automated procedure[1], based on sensitivity analysis for the selection of reactions suitable for optimization and response surfaces method for the search of the best reaction coefficients. In this work a similar procedure has been applied to optimize a gasoline fuel reference mechanism consisting of 1905 reactions and 241 species as developed by Zeuch[2] for the base mechanism (C1-C4) and Ahmed, Blurock and Mauss[3] for larger hydrocarbons following the rules specified by Curran and Westbrook for automatic mechanism generation[4]. This model was used to simulate autoignition in a HCCI engine, using a homogeneous reactor model.

The optimization technique is based on the parameterization of model responses in terms of model parameters by simple algebraic expressions. The ignition delay time, deduced from the pressure profile as the crank angle corresponding to the maximum gradient, was used as optimization target (response). The pre-exponential factors in the reaction's rate Arrhenius expression were chosen as optimization parameters. Second order polynomial expressions were used to map the solution. The interpolation polynomial coefficients were obtained by computer experiments arranged in a fractional factorial design.

**Simulations**. The HCCI-process was modeled as a compressed homogeneous reactor[5]. The EGR was modeled, by running five consecutive engine cycles from Inlet Valve Closing (IVC) at -167 Crank Angle Degree (CAD) to Exhaust Valve Opening (EVO) at 167 CAD. The calculated gas composition at EVO was mixed with the fresh gas composition at IVC. Computations have been carried out on a PC with CPU time requirements of few minutes for each simulation and few hours for a complete optimization process. The entire procedure was performed inside a graphical user interface environment[6]. A sensitivity analysis of the temperature on the Arrhenius coefficients of all reactions included in the kinetic model was performed. The frequency factors of the most sensitive reactions were used as optimization parameters. The selection procedure is visualized in Figure 1. The colors in the graphic indicate the sensitivity level (red, yellow, green, blue, and shades of blue) of the reactions for the cases considered in the calculation.

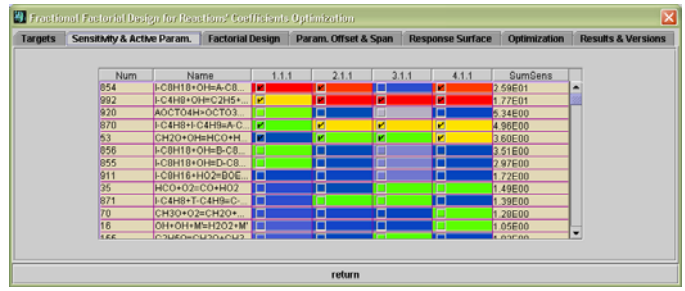


**Figure 1** Screen Snapshot of the Optimization Section of the Graphical User Interface. Selection of Active Optimization Parameters for Each Target.

## Experiments.

The data, needed for the optimization procedure, particularly the ignition delay times, were obtained from experiments conducted at Lund Institute of Technology on a modified Volvo TD100 engine with variable compression ratio and port injection mixes of iso-octane/n-heptane7. A fuel ratio of 0.333 and inlet pressure of 0.9 bars were used. As showed in

Table **1**, a combination of three different inlet temperatures and fuel mixtures was considered, for a total of nine cases. In Table 2 the engines parameters are reported.

**Table 1 Simulations Initial Conditions for: Inlet Temperature, Fuel Mixture and Compression Ratio**

| N | T[K] | Fuel (I-C8H18/N-C7H16) % | CR |
|---|---|---|---|
| 1 | 330 | 100 - 0 | 21.45 |
| 2 | 359 | 100 - 0 | 19.94 |
| 3 | 407 | 100 - 0 | 17.04 |
| 4 | 330 | 83 - 17 | 16.68 |
| 5 | 359 | 83 - 17 | 15.70 |
| 6 | 407 | 83 - 17 | 14.86 |
| 7 | 330 | 51 - 49 | 13.24 |
| 8 | 359 | 51 - 49 | 12.17 |
| 9 | 407 | 51 - 49 | 10.84 |

**Table 2 Engine Parameters**

| | |
|---|---|
| Displaced Volume | 1.602e-3 [m3] |
| Bore | 0.12065 [m] |
| Stroke | 0.14 [m] |
| Rod | 0.26 [m] |
| Speed | 1000 [m/s] |
| Wall Temperature | 490 [K] |
| Start / End DCA | -167 / 167 |
| EGR_Amont | 0.05 [%] |
| EGR Cycles | 5 |

## Results and Discussion

In the framework of this preprint we selected four cases to demonstrate the functionality of the optimization tool (cases 1,2,3 and 6). This gave a reduced system of four targets to be optimized with respect to four reaction rate parameters. The corresponding reactions, their original coefficient and the optimization span, are reported in **Table 3**.

**Table 3 Optimized Reactions**

| N | Name | Original | Optimized | Δ |
|---|---|---|---|---|
| 53 | CH2O+OH=HCO+H2O | 3.4E9 | 2.0E9 | 2 |
| 854 | I-C8H18+OH=A-C8H17+H2O | 1.5E10 | 1.25E10 | 2 |
| 992 | I-C4H8+OH=C2H5+CH3CHO | 1.0E14 | 5.0E13 | 2 |
| 870 | I-C4H8+I-C4H9=A-C8H17 | 8.5E10 | 9.9E10 | 2 |

The pressure profiles for the experimental data compared with those obtained with both the original and optimized model are shown in figure 1-4. For all cases the agreement of the ignition timing with the experiment got improved after the optimization. Shortcomings caused by the simple reactor model, such as to high pressure after ignition, or to short combustion duration can not be improved. The optimization of case 3 is not as good as for the other cases. However, for this case other sensitive reactions (level green in Figure 1) were found. Further optimization runs are prepared that will include these reactions as optimization parameter.

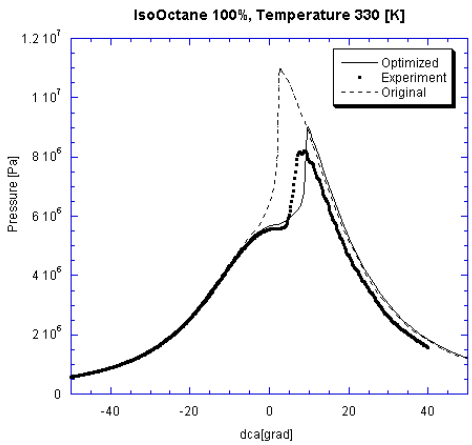


**Figure 2** Pressure Profile vs. Crank Angle Degree for case 1.

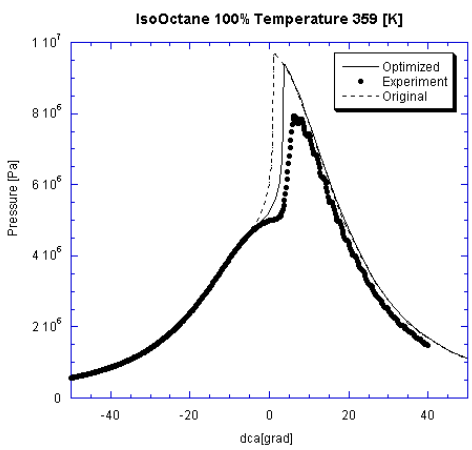


**Figure 3** Pressure Profile vs. Crank Angle Degree for case 2.

## Conclusion

An automatic optimization procedure, based on the solution mapping method, was used to optimize a detailed reaction mechanism for mixtures of n-heptane and iso-octane fuels at varying octane numbers under fuel lean conditions. This was done for HCCI-engine cases, by using a simple compressed reactor model. The optimization target, the maximum pressure rise, was taken from engine experiments. It was shown, that the agreement of mechanism and experiment can be significantly improved, while the effort needed for the procedure is reasonable. Further calculations will be performed, including more engine cases and additional optimization parameters.

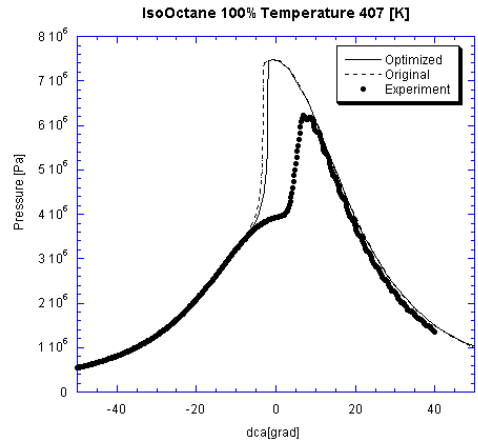


**Figure 4** Pressure Profile vs. Crank Angle Degree for case 3.

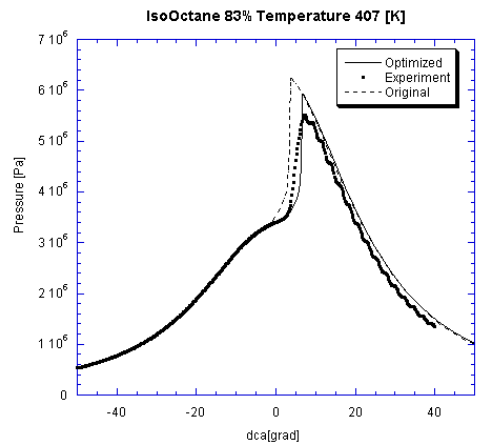


**Figure 5** Pressure Profile vs. Crank Angle Degree for case 4.

## References


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