

# A Global Combustion Model for Simulation of Gasoline HCCI Engines

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## Abstract

A global combustion mechanism was developed for simulation of gasoline self ignition phenomena at engine relevant conditions. This mechanism consists of 14 species and 16 reactions and was validated for different temperatures (650 to 1250 K) and different pressures (10 to 40 bar), using stoichiometric fuel-to-air ratio. The developed model developed was tested for the applicability for simulation of HCCI-engines. Therefore simulation results using different combustion mechanisms were compared. The global model showed good performance for its application to HCCI-engines. The prediction of ignition delay and off-gas species is consistent. More validation has to be done for non-stoichiometric combustion.

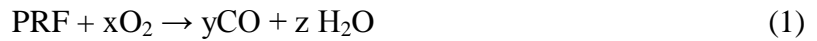
## Background

For the combination of CFD-simulations and combustion chemistry skeletal or even global kinetic models are necessary. As a reason of the huge numbers of species and equations detailed or even semi-detailed combustion mechanisms cause uneconomically long simulation times. The generation of skeletal or global combustion models is always a compromise between excessive numbers of appellative species and a loss of accuracy. In some cases an estimation of the combustion chemistry is sufficient for the whole CFD-simulation. Therefore a global combustion mechanism for gasoline fuels was developed. The main focus was on the simulation of self ignition phenomena and a satisfying calculation of the main combustion products. The validation was done by comparison of different simulation results to literature data and to analog simulations with more detailed combustion mechanisms. More simulations were carried out to demonstrate the applicability of the actual model for calculation of self ignition engines.

## Mechanism development and description

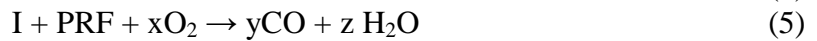
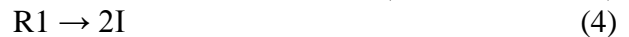
In literature a huge number of combustion mechanisms are published. Whereby most of these are detailed, semi detailed and skeletal kinetic descriptions. Detailed chemistry models are published in [1] to [5]. These models are designed as description of every chemical step taking place during the combustion process, these mechanisms are ideal for validation of the global model. A variety of skeletal mechanisms were developed for the simulation of combustion phenomena implemented to CFD-programs, whereby the focus in these cases is on optimizing combustion processes, or reducing generation of harmful substances. The CFD-simulation is, although the chemistry is already reduced, still very time intensive. For pre-calculations and cases where rough chemistry models are sufficient global combustion mechanisms are preferable. Global combustion kinetics were developed by Zheng et. al [6], and Halstead et al. [7] and other semi-detailed models were developed by many different research groups [8] to [19]. A global model for the prediction of ignition delay times was developed by Müller et. al [20].

As basic set of reactions the mechanism developed by Zheng et. al [6] was taken into account. This model consists of eight global reactions, whereby these reactions and the according kinetic parameters are designed for the calculation of a fixed PRF mixture for gasoline fuels. As surrogates the common substances iso-octane and n-heptane are deployed. In case of the actual research the idea is to simulate different gasoline types by one model, therefore the Zheng model has to be extended. To describe the combustion of different iso-octane and n-heptane mixtures a set of seven additional equations was added. For the simulation of the ignition at different temperatures three different pathways are implemented. For the high temperature ignition the chemical reaction is:



PRF represents either n-heptane or iso-octane or a mixture of both.

For the low temperature ignition the following equations are responsible:



The species R1 represents an oxygenated intermediate radical, and I a chain propagation species. To describe the NTC-region two more equations are added:



These equations are extending the ignition pathway between reaction 3 and reaction 5. By this additional step the thermal runaway is reached later and so the ignition delay time is elongated, what creates the typical maximum in the ignition delay plot (see figure 2). The species R2 can be seen as shifting product of R1.

To fulfill the overall combustion equation for the PRFs the CO generated in reaction 1 and 5 is oxidized to CO<sub>2</sub>:



Reactions 1 to 7 have to exist two times in the combustion mechanism for the two different PRFs with different intermediate species. As a reason of the overestimated water content and temperature in the combustion off-gas found during simulations, another reaction was added. The idea is to shift water with CO to CO<sub>2</sub> and H<sub>2</sub>. In case of this global mechanism the hydrogen chemistry can be excluded, this fact reduces the number of reactions significantly, but on the other hand leads to this water overestimation.



By adding this equation the values of temperature and water content can be corrected. The kinetic parameters were taken out of [21] and adjusted to fit to the whole model.

Reactions of the type 1 to 7 can be found two times in the mechanism description, one time used for the iso-octane and one more time for the n-heptane. On drawback of this model is that no direct interaction between both fuels occurs. That again generates inaccuracies at the

results of ignition delay time simulations. During the ignition process of iso-octane and n-heptane mixtures the starting reactions (type 1 and 2) of both PRFs are running parallel and the thermal runaway is reached, when the ignition of the faster igniting component (n-heptane) occurs. The influence of the iso-octane on the ignition process cannot be calculated by the mechanism in this state. To solve this drawback some kind of interaction has to be implemented, this was done by adding a species-interaction term in the kinetic description of reaction 1 and 2 of n-heptane. This interaction is comparable to the enhanced third body interaction of different species. In this case it has to be a “third body deceleration”, what means if iso-octane is in the fuel mixtures it is decelerating the reaction rates of the n-heptane starting reactions (reaction 1, 2). The mathematic description of the interaction in the reaction-rate equation is:

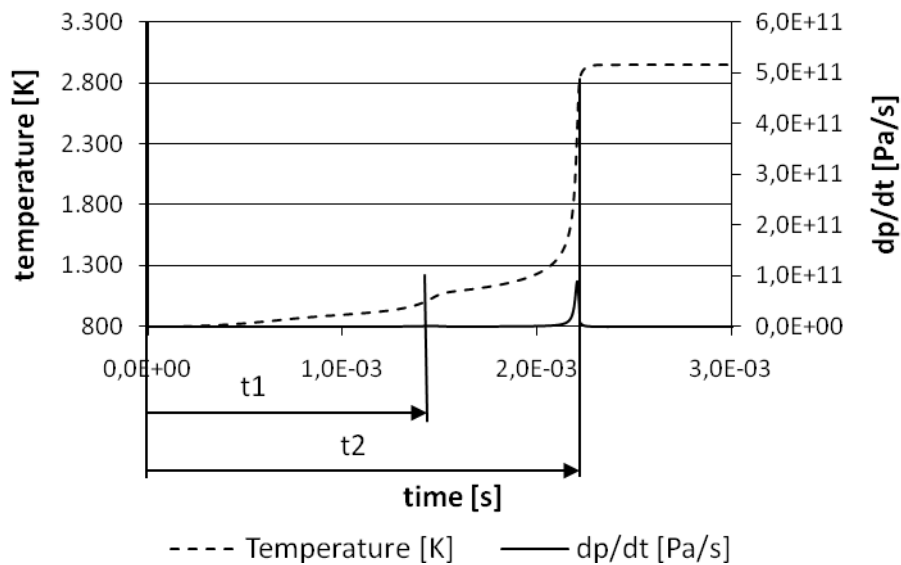
$$R = \left( a_1 \cdot [PRF100] + \sum_{k=2}^K a_k \cdot [X_k] \right) \cdot k \cdot [PRF0]^x \cdot [O_2]^y \quad (10)$$

The reaction rate calculation is illustrated in equation 10, whereby PRF100 represents iso-octane and PRF0 represents n-heptane. The factor  $a$  is an enhancement or in the case of PRF100 a deceleration factor, consequently a negative value. Other species, in this case generally explained by  $X_k$ , are enhanced by a factor  $a=1$ . Of course this deceleration factor is not to be seen like the common enhanced third body interaction, it is a way of fitting a rate expression of a global combustion model.

More details about the developed global combustion mechanism will be published in [22]

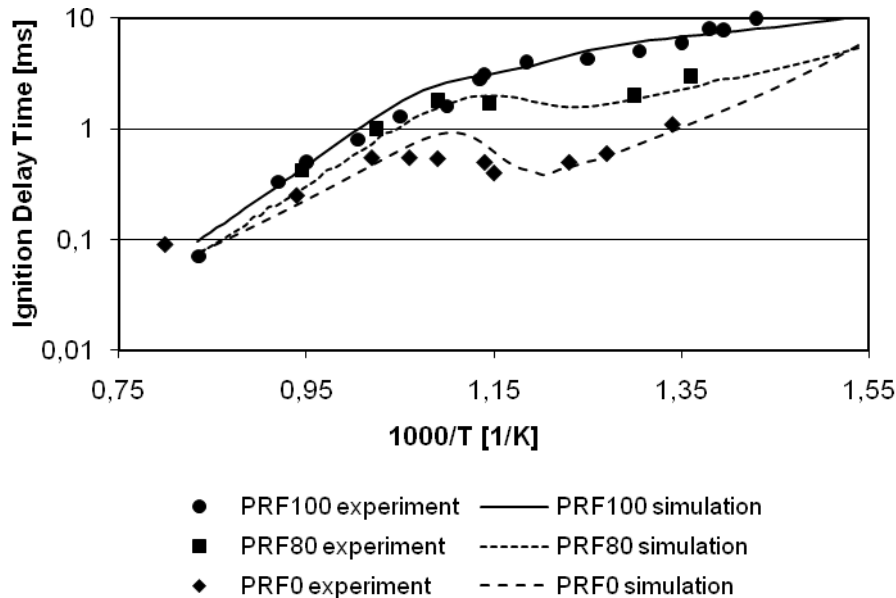
### Validation: ignition phenomena, combustion products

The validation of this combustion mechanism is done by comparing simulation results to literature data [23] [24] or to simulations using more detailed models. During the development process the main focus was on simulation of self ignition phenomena, therefore the ignition delay times of iso-octane, n-heptane and different mixtures of both substances were validated. The validation was done at pressures between 10 and 40 bar and in a temperature region of 650 to 1250K. Simulations were carried out with the program Cosilab, the ignition delay times were calculated using a 0-D model designed for investigation of ignition processes.



**Figure 1.** definition of the ignition delay time

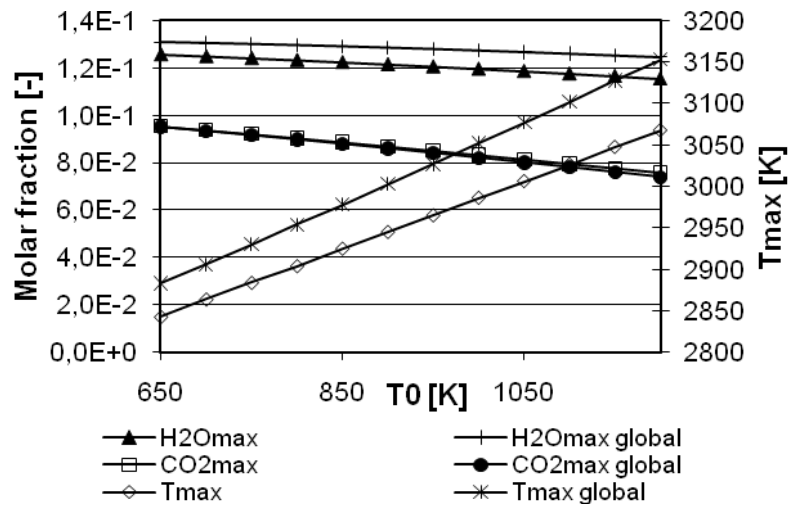
In figure 1 the definition of the ignition delay time can be seen whereby the program Cosilab is able to estimate the ignition point by detecting the maximal  $dT/dt$ ,  $dp/dt$  or a user defined  $\Delta T$ . The time  $t_1$  in figure 1 represents the first stage ignition time and  $t_2$  the ignition delay time of the full ignition process, in all diagrams  $t_2$  is displayed as ignition delay time.



**Figure 2.** ignition delay times of n-heptane (PRF0), iso-octane (PRF100) and a mixture of 80% iso-octane and 20% n-heptane (PRF80) at 40 bar

In figure 2 a comparison of ignition delay times at 40 bar is shown. The experimental values [23] and [24] are compared to simulation results of ignition delay times at different temperatures. More validation for this model was done at lower pressures and for other PRF mixtures at stoichiometric fuel to air ratio. Overall the validation of ignition delay times shows good agreement at different conditions. More validation was done for the off-gas concentrations of the main combustion products like  $CO_2$  and  $H_2O$ , as well as for the occurring combustion temperature. This validation was done comparing results of the actual model to simulations done with other more detailed combustion mechanisms.

The results shown in figure 3 verify the performance of the combustion model, whereby the accordance of the  $CO_2$  mole fractions is excellent, the water mole fractions, as well as the temperature shows some differences. Overall the off-gas composition of the simulation results is acceptable for general combustion applications without focus on harmful substances.



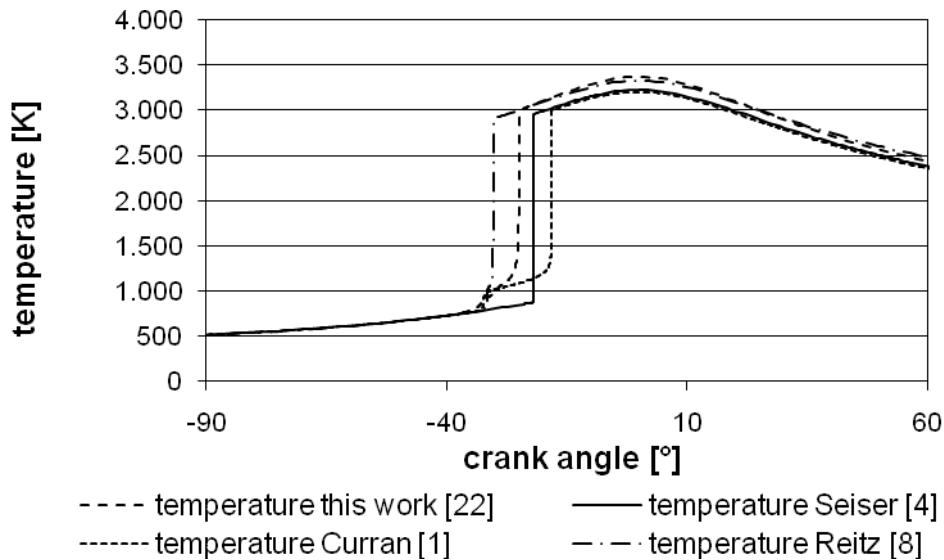
**Figure 3.** comparison of maximum mole fractions of CO<sub>2</sub> and H<sub>2</sub>O and the maximum combustion temperature of stoichiometric n-heptane with simulations of the mechanism [4]

### Simulation: self ignition engine

For more validation different test cases were simulated and compared with a more detailed simulation. A common application for reduced or skeletal combustion mechanism is the simulation of HCCI-engines; therefore calculations at different conditions were carried out using the actual kinetic model and other detailed or reduced mechanisms. The HCCI-engine simulations were carried out using a 0-D HCCI-engine model implemented in the program COSILAB. In table 1 a summary of the simulation conditions is shown:

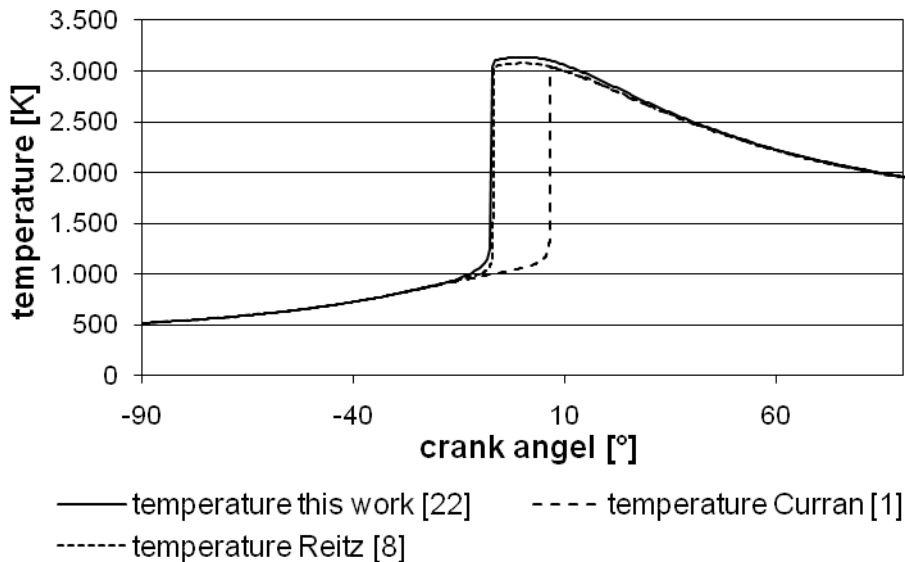
Engine Properties		
Compression ratio	16.5	-
connection-rod length to crank radius ratio	3.71429	-
cylinder volume	0.0001033	m <sup>3</sup>
equivalence ratio	1	-
inlet temperature	447	K
engine speed	1000	rpm

**Table 1.** Parameters of HCCI-engine simulation



**Figure 4.** temperature plot of HCCI-engine simulation for n-heptane using different models [1] (detailed), [4] (semi detailed), [8] (skeletal) and [22] (global)

In figure 4 simulation results of a HCCI-engine are shown. The plot shows, that the temperature calculated using the global mechanism is little overestimated (compared to [1], [4]). The ignition delay time is underestimated compared to [1] and [4] on the other hand it shows an overestimation compared to [8]. Differently compared to [4] the skeletal model is capable to predict first stage ignition affects. Best estimation shows the global model to a skeletal mechanism designed by Ra and Reitz [8]. This model was developed for simulation of HCCI combustion engines.



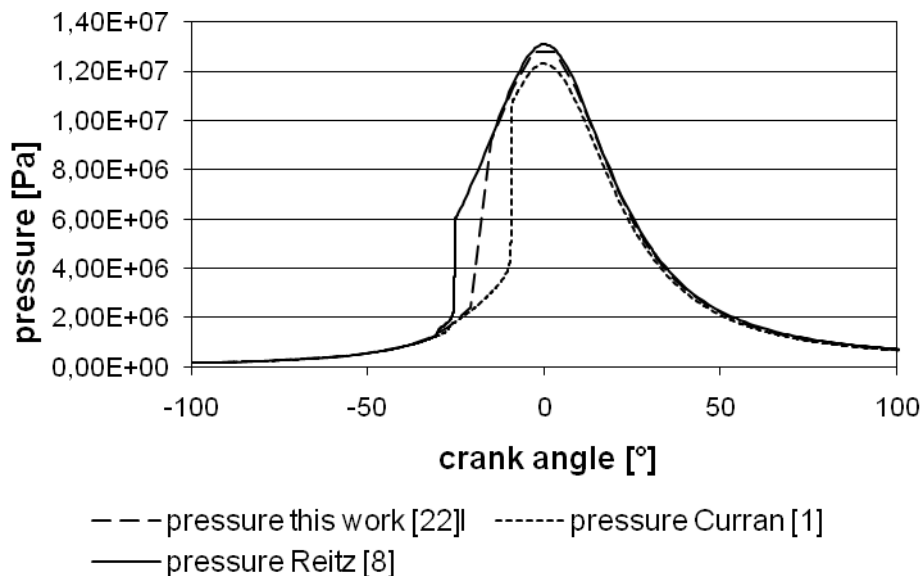
**Figure 5.** temperature plot of HCCI-engine simulation for iso-octane using different models [1] (detailed), [8] (skeletal) and [22] (global)

The comparison of the engine simulations for iso-octane shows good conformance in the temperature prediction (figure 5). The ignition point simulated by the global combustion mechanism is too fast, compared to [1], but is absolutely equal to the simulation using [8], whereby this mechanism is again the one designed for HCCI-engine simulation. More

interesting than the ignition behavior of the pure PRF-substances, is the performance of different mixtures. As described in chapter “mechanism development and description” the interaction between iso-octane and n-heptane is created by deceleration reaction-rates of the ignition reactions. In case of the more detailed models [1] and [8] the interaction is implemented in the mechanism by a huge number of reactions between the intermediate species generated during the ignition process. At the skeletal model for the HCCI-engine simulation this interaction is implemented by a special designed interaction reaction [8]:

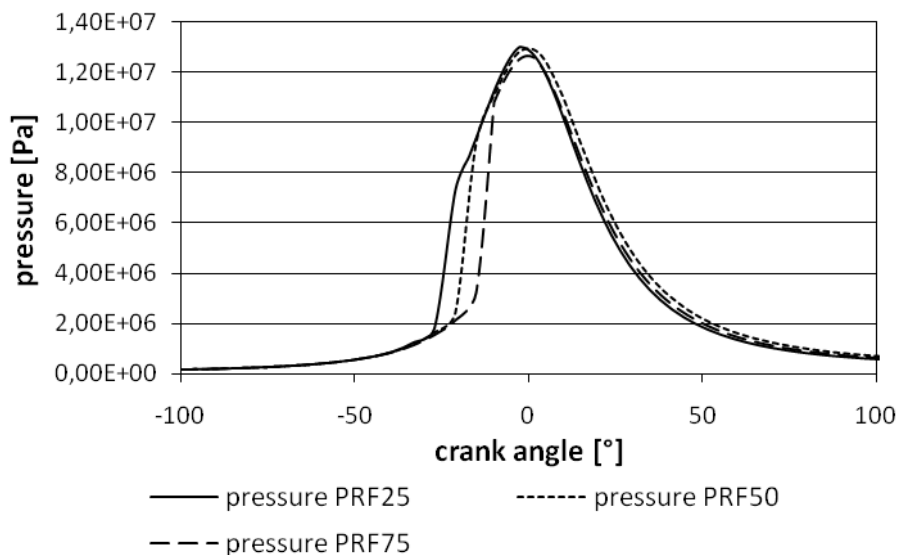


The comparison in figure 6 shows the results of engine simulations using the actual model [22], [1] and [8]. The ignition delay time of the global model is in-between the other used mechanisms, again the estimation of the pressure-plots are good. The peak pressure of the simulated HCCI engine is at about 130 bar, this value goes with experimental data carried out by [17]. The initial values of this experiment are similar to the actual simulations whereby an inlet pressure of 1 bar and a compression ratio of 16 were used. Just the inlet temperature of 318K was lower than in this work.



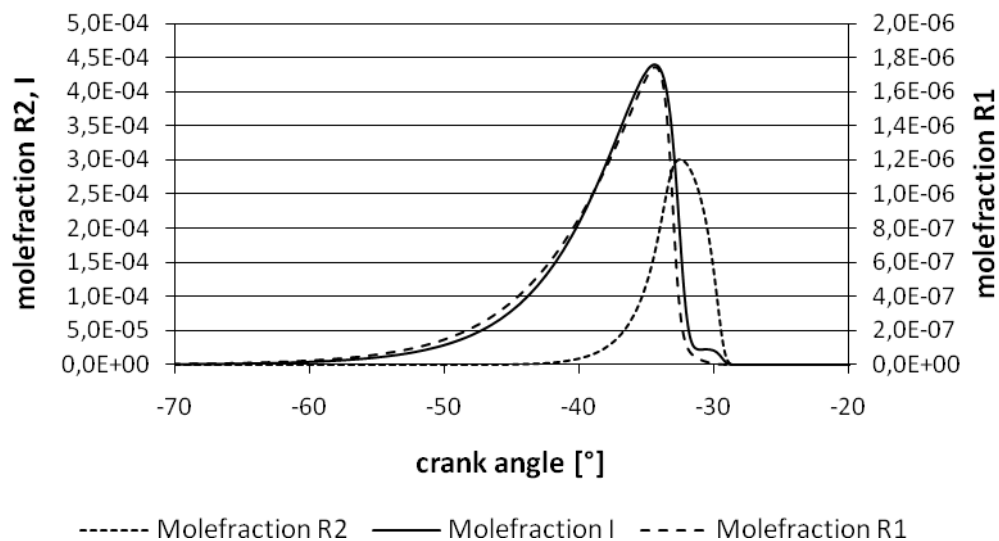
**Figure 6.** comparison of HCCI-engine simulation results using [1] (detailed), [8] (skeletal) and [22] (global)

In figure 7 the change in the ignition points of different n-heptane and iso-octane mixtures is shown. Adding more and more iso-octane to the n-heptane slightly moves the ignition point from about minus 25 to minus 15 degrees crank angle. This shows the way of interaction designed for this model is working; however there are some uncertainties in the simulation of the ignition point compared to the other mechanisms [1], [4] and [8].



**Figure 7.** change of HCCI-engine ignition point, by using different fuel mixtures, PRF25: 25% iso-octane, 75% n-heptane, PRF50: 50% iso-octane, 50% n-heptane, PRF75: 75% iso-octane, 25% n-heptane,

In case of this model there are just six intermediate species describing the whole ignition process, compared to about 30 for [8] and a few hundred for [1]. The intermediates occurring during the n-heptane ignition are shown in figure 8.



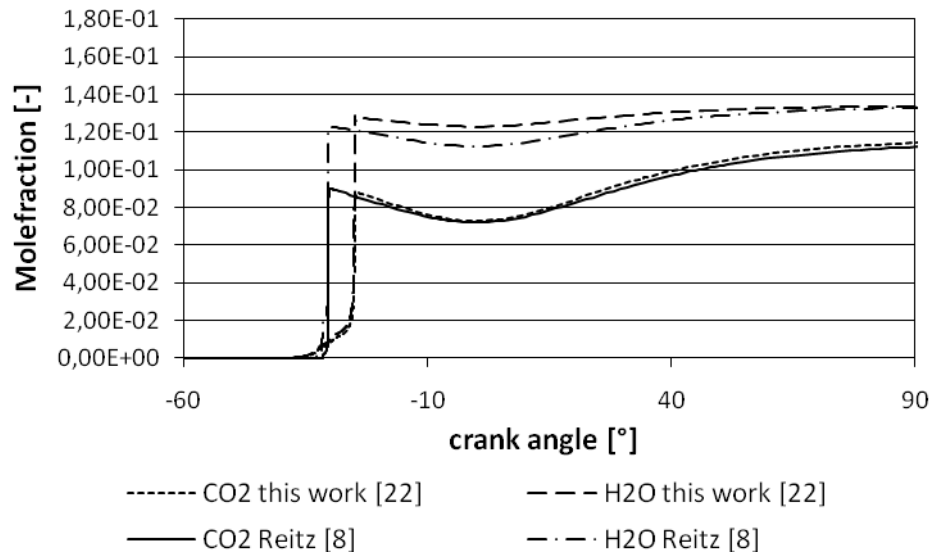
**Figure 8.** Intermediate species occurring during the ignition process of n-heptane.

The ignition process starts with reaction 2, reaction 1 is designed to start at higher temperatures, so in this simulation at the beginning it is of minor importance. R1 is produced by reaction 2 and is consumed by reaction 3 (reverse reaction of 2) and by the reactions 4 and 6. Reaction 4 again is producing the species I (chain propagation species, scission species of R1 and R2). The species I again generates CO and CO<sub>2</sub> in the following reaction 5. The oxidation to CO<sub>2</sub> is generating heat and the following thermal runaway. The rates of the concurring reactions 2 and 3 are responsible for the prediction of the first stage ignition. When the temperature is rising the rate of reaction 3 is getting much faster than the rate of



reaction 2 and the first stage phase passes on to the full ignition stage. Most of R1 is consumed by reaction 4 and smaller amounts by reaction 6; the so generated R2 is again decomposing into I and is delivering heat to the reaction system. This intermediate step is occurring at temperatures between 800 and 1000°C and is responsible for the NTC behavior of the mechanism.

An important requirement of the global model was the simulation of the exhaust gas composition, whereby the focus was on the species H<sub>2</sub>O, CO<sub>2</sub>, CO and H<sub>2</sub>. The simulation of other harmful species or even soot was not taken into account. Figure 9 shows the simulation results of the actual model and [8], again the estimation of the calculated mole fractions is good



**Figure 9.** progress of the off-gas species H<sub>2</sub>O and CO<sub>2</sub>, simulated by [8] (skeletal) and the actual model [22] (global) for n-heptane combustion

As shown above the overall performance of the global model is good, the uncertainties in the ignition delay points compared to other mechanisms are acceptable, because of the global description a certain loss of accuracy is unavoidable. On the other hand the low number of species and equations reduces the simulation time significantly.

## Conclusions

The developed global combustion model consists of 14 species and 16 reactions and is validated for self-ignition phenomena at engine relevant conditions. The validation was done in a temperature region from 650 to 1250 K and for pressures between 10 and 40 bar. The comparison of experimental and simulated ignition delay times showed good agreement for iso-octane, n-heptane and mixtures of both. All the simulations had been done for stoichiometric fuel-to-air ratios; more validation has to be done for non-stoichiometric mixtures.

The simulations of HCCI-engines show good performance. The ignition points and species characteristics are in good accordance to other simulation results using more detailed models. However some uncertainties occurred. As it is described earlier the ignition model for this mechanism is simple. Other mechanisms describe the ignition by using a much higher number of intermediates. These models are able to simulate combustion phenomena much more detailed and the chemistry reproduced is close to the processes running in nature. However,

the aim of this work was to generate a highly reduced model, capable to reflect the major characteristics.

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### Abbreviations, Nomenclature

General:

CFD	computational fluid dynamics
HCCI	homogeneous charge compression ignition
NTC	negative temperature coefficient of ignition delay times
PRF	primary reference fuel

Species:

I	chain branching products of n-heptane/iso-octane
PRF0/PRF100	n-heptane/iso-octane
R1	reaction initiation product of n-heptane/iso-octane
R2	$\beta$ -scission and chain propagation products of n-heptane/iso-octane

Equation parameters:

a [-]	enhancement/deceleration factor
k [*]	rate constant
R [*]	reaction rate
t [s,ms]	time
T [K]	temperature
X	variable species
[X] [mol/m <sup>3</sup> ]	concentration of species X

Indices:

k	number of species
x, y	reaction order

\*...unit defined by equation

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