Modeling and Model-based Control of Homogeneous Charge Compression Ignition (HCCI) Engine Dynamics

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Abstract. The Homogeneous Charge Compression Ignition (HCCI) principle holds promise to increase efficiency and to reduce emissions from internal combustion engines. As HCCI combustion lacks direct ignition timing control and auto-ignition depends on the operating condition, control of auto-ignition is necessary. Since auto-ignition of a homogeneous mixture is very sensitive to operating conditions, a fast combustion phasing control is necessary for reliable operation. To this purpose, HCCI modeling and model-based control with experimental validation were studied. A six-cylinder heavy-duty HCCI engine was controlled on a cycle-to-cycle basis in real time using a variety of sensors, actuators and control structures for control of the HCCI combustion in comparison. The controllers were based on linearizations of a previously presented physical, nonlinear, model of HCCI including cylinder wall temperature dynamics. The control signals were the inlet air temperature and the inlet valve closing. A system for fast thermal management was installed and controlled using mid-ranging control. The resulting control performance was experimentally evaluated in terms of response time and steady-state output variance. For a given operating point, a comparable decrease in steady-state output variance was obtained either by introducing a disturbance model or by changing linearization point. The robustness towards disturbances was investigated as well as the effects of varying the prediction and control horizons. Increasing the horizons had a very limited effect on the closed-loop performance while increasing the computational demands substantially. As shown in the paper, modeling constitutes a necessary element for embedded networked control design applied to HCCI combustion engine design.

1 Introduction

The motivation for studying the homogeneous charge compression ignition (HCCI) engine principle is the promise of low levels of exhaust emissions with regards to NO_x, while still retaining an acceptable overall efficiency [15]. Pioneering efforts towards this new engine principle—also called controlled auto-ignition (CAI)—were reported in [42, 57, 21, 14, 30]. Depending on the purpose, modeling of HCCI engine dynamics may exhibit different complexity and format such as:

– Multi-zone models including chemical kinetics to simulate engine operation in a large operating range;

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– Multidimensional CFD for optimization of fuel injection and combustion chamber design;
– Single-zone reduced-order dynamic models (for model-based control).

A significant challenge with HCCI is the control of the combustion phasing, this is essential in order to control the load, to obtain low fuel consumption and emissions. For closed-loop control of the combustion phasing, feedback signals are necessary and in-cylinder pressure feedback is, perhaps, the most straightforward approach. In practice, the crank angle α of 50% burnt fuel (CA50 or α_{50} or θ_{50}) has proved to be a reliable indicator of on-going combustion [41, 6]. In closed-loop control of an HCCI engine, several means to actuate the combustion phasing have been tested—*e.g.*, dual fuels [41, 6, 8], variable valve actuation (VVA) [1, 8], variable compression ratio [15, 27], and thermal management [38, 28].

For control design purposes and embedded control design exploiting information from networked sensors, appropriate models and system variables useful for feedback control are needed. Previously, it was shown that physical modeling and system identification can be used to obtain low-complexity models of the HCCI dynamics [58, 7, 51]. For closed-loop HCCI engine operation, it was reported that the combustion phasing can be stabilized by means of a PID controller [41]; LQG control [58]; and MPC control [8].

A fast and robust control of α_{50} appears to be necessary in order to stabilize HCCI engine control. It is also desirable that the load, peak cylinder pressure, peak rate of cylinder pressure and emissions are controlled simultaneously. This is a multi-input multi-output (MIMO) control problem where the controller has to be able to handle constraints on several variables. In a comparison among several control methods, it will be demonstrated that Model Predictive Control (MPC) control could be used with favorable properties [4, 35]. All of the actuators suggested have control constraints and MPC has the benefit of explicitly taking the constraints into account.

Whereas monitoring of α_{50} or other methods to sense on-going combustion for feedback control of an HCCI engine all rely on pressure sensors, these sensors may be expensive. One candidate to replace pressure sensors is the use of electronic conductive properties for the reaction zone [24]. This phenomenon is called ion current for which no expensive sensor is needed. Ion current has been successfully used in closed-loop control of SI engines [20]. The basic principle of ion current sensing is that a voltage is applied over an electrode gap inserted into the gas volume (combustion chamber) [24]. The common belief so far has been that ion current levels are not measurable for the highly diluted HCCI combustion. However, a recent study shows that it is not the dilution level in itself but the actual fuel/air equivalence ratio ϕ which is an important factor for the signal level [22, 58].

In this paper, we will report new modeling and experimental results on HCCI control, complementing our previously published results on control of a six-cylinder heavy-duty engine, evaluating a variety of control methods (MPC and PID) and actuators (VVA, dual fuel), and experimental results on HCCI control of a single-cylinder heavy-duty engine evaluating a variety of sensors (in-cylinder pressure, ion current) [8, 9, 7].

The purpose of this paper is to provide a survey of state-of-the-art HCCI engine modeling with particular attention to control-oriented modeling relevant for networked

embedded system design. The structure of the paper is the following: An overview of HCCI modeling is given with particular emphasis on modeling suitable for model-based control, followed by a model-based control description, discussion and conclusions.

2 HCCI Modeling

There are two often used methods to obtain models of HCCI engine dynamics suitable for control; physical modeling [51] and modeling by means of system identification [7–9]. Physical modeling based on conservation laws and chemical kinetics has attractive intuitive component-based features but suffers from complexity issues with adverse effects in application. Whereas system identification has proved to be a very effective modeling tool for prototyping, it may provide results hard to interpret from a physical point of of view.

The purpose of modeling has an obvious influence on focus and the complexity of modeling [33, 19]. As modeling and simulation may easily become too detailed and computationally expensive to serve purposes of model-based control, low-complexity models and reduced-order models become relevant. A minimum requirement of physical modeling is explanation of the nature of the in-cylinder pressure traces where adiabatic compression combines with fuel-dependent auto-ignition [43], [10], [23]. In previous work, modeling choices involve aspects of chemical kinetics, cycle-to-cycle coupling, in-cylinder concentrations of reactants, wall temperature dynamics, pressure dynamics, and auto-ignition timing.

Modeling details fall into categories of single-zone models, multi-zone models, multidimensional computational fluid dynamics (CFD) models, sometimes combined with exosystem simulation on the form of stochastic disturbances, load modeling, sensor modeling. Both physical aspects and operational aspects require attention. Shaver *et al.* singled out six distinct stages in modeling of HCCI engine operation—*i.e.*, induction, compression, combustion, expansion, exhaust and residence in the exhaust manifold [52, 53, 45]. As for stable operation, combustion phasing control design requires appropriate models and system output variables usable for feedback control. Recently, mode-transition operation and control of Diesel-HCCI and SI-HCCI engines and other hybrid control aspects have received attention [54].

2.1 Fuel Modeling

The necessity of developing a practical iso-octane mechanism for HCCI engines was presented after various different experiments and currently available mechanisms for iso-octane oxidation being reviewed and the performance of these mechanisms applied to experiments relevant to HCCI engines being analyzed [48, 39]. A skeletal mechanism including 38 species and 69 reactions was developed, which could predict satisfactorily ignition timing, burn rate and the emissions of HC, CO and NO_x for HCCI multi-dimensional modeling [39]. Comparisons with various experiment data including shock tube, rapid compression machine, jet-stirred reactor and HCCI engine indicate good performance of this mechanism over wide ranges of temperature, pressure and equivalence ratio, especially at high pressure and lean equivalence ratio conditions. By

applying the skeletal mechanism to a single-zone model of an HCCI engine, it was found that the results were substantially identical with those from the detailed mechanism developed by Curran et al. [18] but the computing time was reduced greatly [39].

A model for the auto-ignition of hydrocarbons applicable to 3D internal combustion engine calculations was proposed [16]. The limits of classical methods using an auto-ignition delay are investigated when cool flame phenomena are present. A method based on tabulated reaction rates was presented to capture the early heat release induced by low temperature combustion. Cool flame ignition delay when present and cool flame fuel consumption are also tabulated. The reaction rate, fuel consumption, and cool flame ignition delay tables were built a priori from complex chemistry calculations. The reaction rates, which directly depend on instantaneous changes of thermodynamic conditions, were then integrated during the 3D engine calculation. The model is first validated through comparisons with complex chemistry calculations in constant and variable volume configurations where good agreement was found. The model was applied both to a Diesel computation with spray injection and residual gases, and to a Diesel-HCCI configuration. Comparisons with experimental results showed that the auto-ignition essential features were well reproduced in these cases [16].

The combination of CFD computations with detailed chemistry leads to excessive computation times, and is not achievable with current computer capabilities. A reduced chemical model for $n-$heptane is described, in view of its implementation into a CFD simulation code [37]. Firstly, the reduction process to get to the 61-step mechanism is detailed and then the 26-step mechanism is described; this further reduction is carried out under various conditions that include a range of interest in engine applications. Validation work in reference to the original detailed mechanism and two reduced mechanisms was published in the literature, focusing on the prediction of ignition delay times under constant as well as variable volume conditions [37]. A good and accurate reproduction of both ignition delay times and heat release was reported to be reached with the 26-step model [37].

Despite the rapid combustion typically experienced in HCCI, components in fuel mixtures do not ignite in unison or burn equally. In experiments and modeling of blends of diethyl ether (DEE) and ethanol, the DEE led combustion and proceeded further toward completion, as indicated by ^{14}C-isotope tracing [36]. A numerical model of HCCI combustion of DEE and ethanol mixtures supports the isotopic findings. Although both approaches lacked information on incompletely combusted intermediates plentiful in HCCI emissions, the numerical model and ^{14}C-tracing data agreed within the limitations of the single-zone model. Despite the fact that DEE is more reactive than ethanol in HCCI engines, they were sufficiently similar and prevented incidence of a large elongation of energy release or significant reduction in inlet temperature required for light-off, both desired effects for the combustion event. This finding suggests that, in general, HCCI combustion of fuel blends may have preferential combustion of some of the blend components [36].

2.2 Auto-Ignition Modeling

Whereas HCCI engines have been shown to have higher thermal efficiencies and lower NO_x and soot emissions than spark ignition engines, the HCCI engines experience very

large heat release rates which can cause too rapid an increase in pressure. One method of reducing the maximum heat-release rate is to introduce thermal inhomogeneities, thereby spreading the heat release over several crank angle degrees [55]. Direct numerical simulations (DNS) showed that both ignition fronts and deflagration-like fronts may be present in systems with such inhomogeneities [17]. Here, an enthalpy-based flamelet model was presented and applied to four cases of varying initial temperature variance. This model used a mean scalar dissipation rate to model mixing between regions of higher and lower enthalpies. The predicted heat-release rates agree well with the heat release rates of the four DNS cases. The model was shown to be capable of capturing the combustion characteristics for the case in which combustion occurs primarily in the form of spontaneous ignition fronts, for the case dominated by deflagration-type burning, and for the mixed mode cases. The enthalpy-based flamelet model shows considerably improved agreement with the DNS results over the popular multi-zone model, particularly, where both deflagrative and spontaneous ignition are occurring, that is, where diffusive transport is important [17]. Another fuel model is the Shell model used for auto-ignition below [26]. Further contributions on auto-ignition modeling can be found in [47].

2.3 Thermal Modeling and Auto-Ignition

HCCI combustion is often achieved without a completely homogeneous mixture. In order to derive a control-relevant model, however, we might firstly proceed by assuming that the mixture is homogeneous, thus allowing a single-zone cylinder model [5]. Such assumptions may be justified by laser-diagnostic measurements in our experimental set-up [46]. To reproduce the effects relevant for combustion phasing control it is required that the auto-ignition model captures the effects on ignition delay (induction time) of varying species concentrations, temperature trace, and fuel quality. Several alternative approaches are possible for modeling the instant of auto-ignition for fuels. High-complexity models—*e.g.*, (Primary Reference Fuels (PRF), 857 species, 3,606 reactions, CHEMKIN/LLNL) [56]—have been used to model complete combustion. In addition to ignition prediction, such models are also aimed at describing intermediate species and end product composition. Reduced chemical kinetics models, *e.g.*, (PRF fuels, 32 species, 55 reactions, CHEMKIN) [60], have also been proposed, where reactions with little influence on the combustion have been identified and removed. For simulation of multi-cycle scenarios it is necessary to keep the model complexity low in order to arrive at reasonable simulation times. An attractive and widespread alternative is to use the Shell model [26], which is a lumped chemical kinetics model using only five representative species in eight generic reactions. This model is aimed at prediction of auto-ignition rather than describing the complete combustion process. Compression ignition delay may also be described by empirical correlations, such as the *knock integral* condition

$$\int_{t=0}^{t_i} \frac{dt}{\tau} = 1 \tag{1}$$

where t_i is the instant of ignition and τ is the estimated ignition time (ignition delay) at the instantaneous pressure and temperature conditions at time t, often described by

Arrhenius type expressions [29, 49]. A drawback is that dependence on species concentrations is normally not regarded. An integral condition with concentration dependence was used in [50, 51] in a similar study for propane fuel, where also auto-ignition models based on very simple reaction mechanisms were evaluated. Alternatives to physical or physics-based models are to use system identification to obtain models or to use empirical look-up tables. The latter gives insufficient physical insight, and require substantial efforts to calibrate. In this work, the Shell model was chosen to describe the process of auto-ignition. A static model is then used to describe the major part of the actual combustion and corresponding heat release. The result from the Shell model was compared to results from an integrated Arrhenius rate threshold model and the Planet mechanism model [3, 2]. To the purpose of detailed treatise, modeling of the cylinder, auto-ignition, integrated Arrhenius threshold, combustion, and heat transfer are now provided:

Cylinder Gas Model—First Law of Thermodynamics. The cylinder gas dynamics are described by conservation laws such as the the first law of thermodynamics

$$\delta Q_{HR} = (1 + \frac{c_v}{R})p\mathrm{dV} + \frac{c_v}{R}V\mathrm{dp} + \delta Q_{HT} \tag{2}$$

where p is the cylinder pressure, V the volume, R_u the universal gas constant, $c_v = c_p - R_u$ the specific heat capacity, and n the molar substance amount contained in the cylinder. The time derivatives of Q_{HR} and Q_{HT} denote rates of heat released by the combustion process and heat flowing from the wall, respectively.

Gas Properties. The gas is described as a mixture of dry air and fuel, and the combustion products are nitrogen, carbondioxide and water. Specific heat for each species i is described by NASA polynomial approximations of JANAF data

$$c_{p,i}(T) = \frac{R_u}{M_i}\sum_{j=1}^{5} a_{i,j}T^{j-3} \tag{3}$$

where M_i is the molar mass of species i and T is the cylinder temperature [12, 25]. The mixture specific heat is then

$$c_p(T) = \frac{1}{n}\sum_i n_i M_i c_{p,i}(T) \tag{4}$$

where n_i is the mole of species i.

Shell Auto-ignition Model. The Shell auto-ignition model for hydrocarbon fuels [26], C_aH_b, is based on a general eight-step chain-branching reaction scheme with lumped species: The hydrocarbon fuel RH, radicals $\bar{R}$, intermediate species Q, and the chain branching agent B.

$$RH + O_2 \xrightarrow{k_q} 2\bar{R} \quad \text{(initiation)} \tag{5}$$

$$\bar{R} \xrightarrow{k_p} \bar{R} + \text{products and heat} \quad \text{(propagation cycle)} \tag{6}$$

$$\bar{R} \xrightarrow{f_1 k_p} \bar{R} + B \quad \text{(propagation forming } B\text{)} \tag{7}$$

$$\bar{R} + Q \xrightarrow{f_2 k_p} \bar{R} + B \quad \text{(propagation forming } B\text{)} \tag{8}$$

$$\bar{R} \xrightarrow{f_3 k_p} \text{out} \quad \text{(linear termination)} \tag{9}$$

$$\bar{R} \xrightarrow{f_4 k_p} \bar{R} + Q \quad \text{(propagation forming } Q\text{)} \tag{10}$$

$$2\bar{R} \xrightarrow{k_t} \text{out} \quad \text{(quadratic termination)} \tag{11}$$

$$B \xrightarrow{k_b} 2\bar{R} \quad \text{(degenerate branching)} \tag{12}$$

Auto-ignition is described by integrating the time variations of species concentrations from the beginning of the compression stroke.

$$\frac{d[\bar{R}]}{dt} = 2\left\{k_q[RH][O_2] + k_b[B] - k_t[\bar{R}]^2\right\} - f_3 k_p[\bar{R}] \tag{13}$$

$$\frac{d[B]}{dt} = f_1 k_p[\bar{R}] + f_2 k_p[Q][\bar{R}] - k_b[B] \tag{14}$$

$$\frac{d[Q]}{dt} = f_4 k_p[\bar{R}] - f_2 k_p[Q][\bar{R}] \tag{15}$$

$$\frac{d[O_2]}{dt} = -g k_p[\bar{R}] \tag{16}$$

The species $\bar{R}$, Q, and B are not considered in thermodynamic computations for the gas mixture. The stoichiometry is approximated by assuming a constant CO/CO_2 ratio, ν, for the complete combustion process, with oxygen consumption $g = 2[a(1-\nu)+b/4]/b$ mole per cycle. The heat release from combustion is given by

$$\frac{dQ_{HR}}{dt} = k_p q V[\bar{R}] \tag{17}$$

where q is the exothermicity per cycle for the regarded fuel. The propagation rate coefficient is described as

$$k_p = \left(\frac{1}{k_{p,1}[O_2]} + \frac{1}{k_{p,2}} + \frac{1}{k_{p,1}[RH]}\right)^{-1} \tag{18}$$

To capture dependence of induction periods on fuel and air concentrations the terms f_1, f_3, and f_4 are expressed as

$$f_i = f_i^{\circ}[O_2]^{x_i}[RH]^{y_i} \tag{19}$$

Rate coefficients and rate parameters k_i and f_i° are then described by Arrhenius rate coefficients

$$k_i = A_i \exp\left[\frac{-E_i}{R_u T}\right], \quad f_i^{\circ} = A_i \exp\left[\frac{-E_i}{R_u T}\right] \tag{20}$$

We use the acronym FuelMEP to denote the mean effective pressure calculated from the quantity of fuel injected. Calibrated parameters for a number of fuels, including a set of Primary Reference Fuels (PRF), are found in the literature [26]. PRFx is a mixture of n-heptane and iso-octane, where the octane number x is defined as the volume percentage of iso-octane. Parameters for PRF90 were used in the simulations. Auto-ignition was defined as the crank angle where the explosive phase of combustion starts.

Integrated Arrhenius Rate Threshold. The Arrhenius form can be used to determine the rate coefficient describing a single-step reaction between two molecules [62]. The single-step rate integral condition is based on the knock integral with

$$K_{th} = \int_{\theta_{\mathrm{IVC}}}^{\theta} 1/\tau \; d\theta/w \tag{21}$$

$$1/\tau = A \exp(-E_a/(R_u T))[\mathrm{Fuel}]^a [O_2]^b \tag{22}$$

where θ is the crank angle and θ_{IVC} is the crank angle of the inlet valve closure. The integral condition describes a generalized reaction of fuel and oxygen and this is an extreme simplification of the large number of reactions that take place during combustion. The empirical parameters A, E_a, a, b and K_{th} are determined from experiments. Values for n-heptane and iso-octane from [62] were used in the comparison below with $A = 4.65 \cdot 10^{11}$, $E_a = 15.1$, $a = 0.25$, $b = 1.5$, $K = 1.6 \cdot 10^5$. Auto-ignition was defined as the crank angle where the integral condition has reached the threshold K_{th}. Sensitivity analysis of integrated Arrhenius rate thresholding was made by Chiang and Stefanoupolou [32].

Combustion. When auto-ignition is detected by the Shell model or the Integrated Arrhenius Rate Threshold, the completion of combustion is described by a Wiebe function [65].

$$x_b(\theta) = 1 - \exp\left[-a(\frac{\theta - \theta_0}{\Delta\theta})^{m+1}\right] \tag{23}$$

where x_b denotes the mass fraction burnt, θ is the crank angle, θ_0 start of combustion, $\Delta\theta$ is the total duration, and a and m adjustable parameters that fix the shape of the curve. The heat release is computed from the rate of x_b and the higher heating value of the fuel.

Heat Transfer. Heat is transfered by convection and radiation between in-cylinder gases and cylinder head, valves, cylinder walls, and piston during the engine cycle. In this case the radiation is neglected. This problem is very complex, but a standard solution is to use the Newton law for external heat transfer

$$\frac{dQ_W}{dt} = h_c A_W (T - T_W) \tag{24}$$

where Q_W is the heat transfer by conduction, A_W the wall area, T_W the wall temperature, and the heat-transfer coefficient h_c given by the Nusselt-Reynolds relation by Woschni [66]

$$h_c = 3.26 B^{-0.2} p^{0.8} T^{-0.55} (2.28 S_p)^{0.8} \tag{25}$$

where S_p is the mean piston speed and B is the bore.

3 Experiments

Detailed reviews of experimental set-up and conditions are given in [8, 9, 11].

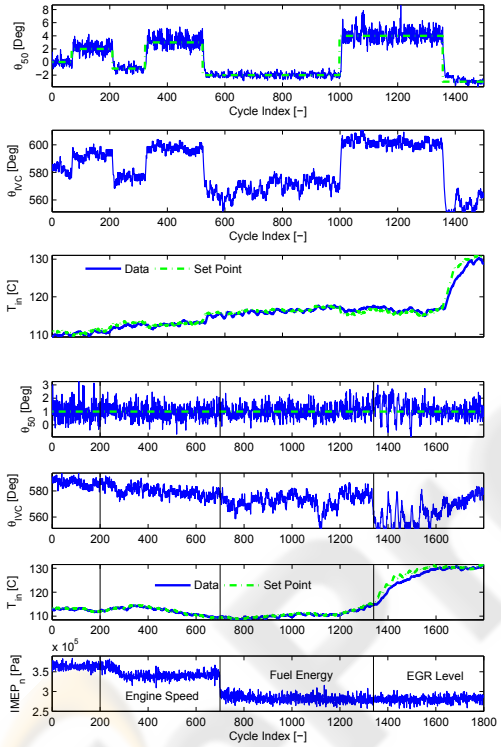

Fig. 1. Results of consecutive set-point changes (*upper*) and response to disturbances (*lower*) [63].

A cycle-resolved model of HCCI presented in [64] was used to design model predictive controllers. The controlled output was the crank angle of 50 % burnt fuel (here denoted θ_{50}). The control signals were the inlet air temperature and the crank angle of inlet valve closing. A fast thermal management system was used to obtain fast intake temperature actuation.

As witnessed by Fig 1, successful model-based control was accomplished both for setpoint tracking and disturbance rejection.

4 Conclusions

In addition to aspects of modeling related to thermodynamics, chemical combustion kinetics, and engine operation, careful attention is required for control-oriented com-

bustion modeling and the interactions among dynamics, control, thermodynamics and chemical combustion properties. Modeling of engine-load transients as well as thermal transients also belong to this important domain of modeling (Fig. 1). Progress in this area is important and necessary for successful and robust control such as model-predictive control.

Within the project a cycle-resolved, physics-based, model of HCCI has been developed. The model includes a low-complexity model of the cylinder wall temperature dynamics in order to capture the relevant time-scales of transient HCCI when only small amounts of hot residuals are trapped in the cylinder. The temperature evolution of the gas charge is modeled as isentropic compression and expansion with three heat transfer events during each cycle.

Recently, research focused on design and evaluation of model predictive controllers based on linearizations of the model. The considered control signals were the inlet valve closing and the intake temperature. Simulations were used for the initial control design and the resulting controller was tested experimentally. The control performance was evaluated in terms of response time to set-point changes and the resulting output variance.

It was found that a comparable decrease in the output variance in some operating points could be achieved either by introducing a disturbance model or by changing linearization. All tested set-point changes were accomplished within 20 engine cycles or less. Only minor changes to the intake temperature were required for moderate changes. The closed-loop system showed good robustness towards disturbances in engine speed, injected fuel energy, and the amount of recycled exhaust gases.

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