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A PHYSICALLY BASED TWO-STATE MODEL FOR CONTROLLING EXHAUST RECOMPRESSION HCCI IN GASOLINE ENGINES

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ABSTRACT

Homogeneous Charge Compression Ignition (HCCI) presents several advantages over conventional IC engines, including improved efficiency and emissions. It is, however, difficult to implement and control due to the lack of an external combustion trigger. One way to achieve HCCI is to trap and re-compress a portion of the exhaust in the cylinder to increase the sensible energy of the air-fuel mixture. Such a strategy, however, introduces a cyclic coupling through the exhaust gas retained from cycle to cycle, making dynamic control non-trivial. In order to develop model-based controllers for HCCI, the authors present a physically motivated two-state model of the HCCI process. This model specifically captures the behavior of a direct inject gasoline engine with an exhaust-recompression strategy used to achieve HCCI. As the trapped exhaust is pivotal in setting up the cyclic coupling, its temperature and the amount of oxygen present in it are selected as the states of the system. The system's dynamics are developed through these states to give a discrete-time nonlinear model that can be validated against a more complex continuous-time model. In this form, the model represents a control-oriented description of the HCCI engine as a thermodynamic system, and can therefore be used as a platform to synthesize various control strategies. As a demonstrative example, a linear representation of the system is derived and used to synthesize an LQR controller to track a desired state trajectory in simulation.

NOMENCLATURE

A_{th}	Arrhenius rate pre-exponential factor
$\bar{C}_p$	Constant average specific heat (at constant pressure) for cylinder contents
$\bar{C}_v$	Constant average specific heat (at constant volume) for cylinder contents
$\bar{C}_{v,f}$	Specific heat (at constant volume) for fuel
γ	Specific heat ratio
E_a	Activation energy for gasoline
EVO	Exhaust Valve Opening time
EVC	Exhaust Valve Closing time
ε	Fraction of fuel LHV representing heat loss during combustion

h_{fg}	Enthalpy of vaporization of fuel
IVO	Intake Valve Opening time
IVC	Intake Valve Closing time
K_{th}	Arrhenius threshold value
LHV_f	Lower heating value of fuel
$n_{a,k}$	Moles of fresh air inducted into cylinder during engine cycle k
$n_{e,k}$	Moles of exhaust trapped in cylinder at EVC during engine cycle k
$n_{f,k}$	Moles of fuel injected into cylinder during engine cycle k
$n_{O_2,k}$	Moles of oxygen trapped in cylinder at EVC for engine cycle k
P_{atm}	Atmospheric pressure
$P_{i,k}$	Pressure at which fresh air is inducted into the cylinder
$P_{j,k}$	Pressure following stage j for engine cycle k (j=1,...,5)
R_u	Universal Gas Constant
ψ_k	Fraction of external EGR for engine cycle k
$T_{e,k}$	Temperature of trapped exhaust at EVC for engine cycle k
$T_{j,k}$	Temperature following stage j for engine cycle k (j=1,...,5)
$V_{j,k}$	Cylinder volume following stage j for engine cycle k (j=1,...,5)
$V_{IVC,k}$	Cylinder volume at IVC for engine cycle k
$V_{EVC,k}$	Cylinder volume at EVC for engine cycle k
$V_{23,k}$	Cylinder volume at combustion event for engine cycle k
ω_k	Engine speed in cycle k
χ	Fractional change in temperature of trapped exhaust during recompression
$\bar{}$	Value of a quantity at nominal operating condition
$\hat{}$	Deviation of a quantity from nominal operating condition

INTRODUCTION

Homogeneous Charge Compression Ignition (HCCI) engines represent the next generation in IC engine technologies, providing significantly better fuel efficiency and emissions characteristics than engines today. In particular, they have dramatically low NO_x emissions [1]. HCCI is achieved by compressed auto-ignition of a homogeneous fuel/air mixture, which is possible when the sensible energy of the reactant charge is increased. There are several ways in which this increase in sensible energy can be achieved. The inducted air can be heated or pre-compressed [2, 3] in order to increase its energy. Alternately, hot exhaust gases can be mixed with fresh charge to obtain a mixture with higher sensible energy. Such a strategy is known as *residual-affected HCCI*. Residual-affected HCCI can be achieved with a variable-valve actuation system in several ways. One method is to use a delayed closing of the exhaust valve to *reinduct* some of the exhaust from the exhaust manifold [1, 4]. Alternately, in what is known as *Recompression HCCI*, the exhaust valve is closed early, trapping some of the exhaust within the engine cylinder, which gets recompressed as the piston continues its upward stroke [4].

There are however significant challenges in implementing HCCI in practice. Unlike spark and compression ignition engines, where the combustion is initiated respectively by a spark and the injection of diesel fuel, the combustion in an HCCI engine is more directly governed by the characteristics of the mixture in the cylinder and reaction kinetics. Therefore there is no external combustion trigger for the process. In addition, in the case of residual-affected HCCI, the exhaust that is carried through from one engine cycle to the next induces a cyclic coupling that complicates both steady-state and transient operation. Therefore, in order to achieve and maintain stable HCCI, closed-loop control strategies are necessary.

A first step towards this is the synthesis of a model of the HCCI process. Several approaches to this end have been proposed. These range from simple zero-dimensional models (the earliest example of these being proposed by Najt et.al [5]) to those with more detailed chemical kinetics and thermodynamics [6–8]), to multi-dimensional CFD models [9]. However, for the synthesis of model-based controllers we require models that are simple, but still capture the key dynamics of the HCCI process. Such a model is presented in previous work by Shaver et. al [10, 11]. This model captured the behavior of a propane-fueled HCCI engine with exhaust reinduction, and was shown to be suitable for designing controllers. However, it is only applicable to the particular HCCI strategy being modeled, and is not easily generalizable. The inputs to the model - effective compression ratio and the ratio of fresh charge and exhaust - are abstracted from the actual physical inputs available - valve timings. Therefore the model is a step removed from implementation. However, with a static map from valve timings to the model inputs, effective closed-loop control of HCCI was demonstrated in experiment.

The key thrust of the work presented in this paper is to develop a model of HCCI suitable for controller development, based on a fundamental description of HCCI thermodynamics. The model states are chosen so as to represent physical quantities critical in determining the nature of HCCI combustion - reactant concentrations and temperature [6]. Based on this, a recompression HCCI strategy with direct-inject gasoline is modeled. As the role of the trapped exhaust in establishing the cyclic coupling, and influencing combustion is critical, the states for the model are chosen as the moles of oxygen in the trapped exhaust, the temperature of the trapped exhaust. A discrete time approach is used to model HCCI dynamics from one engine cycle to the next, by breaking up a single HCCI cycle into several well defined stages. The engine as a thermodynamic system is therefore modeled from a controls perspective, providing a valuable tool for controller synthesis. This nonlinear model is validated in simulation against a more complex continuous-time model of HCCI presented in [7]. To demonstrate the model's efficacy as a tool for controller synthesis, it is linearized about an operating point and used to synthesize an LQR controller. When tested in

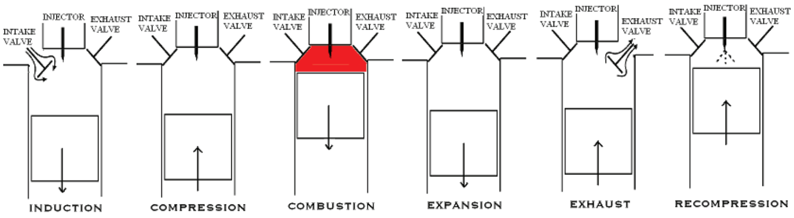

Figure 1. Breakdown of an HCCI engine cycle

simulation, the controller tracks the desired trajectory accurately.

MODEL DESCRIPTION

A typical HCCI engine cycle with exhaust recompression, and direct fuel injection can be described as shown in Figure 1. The intake valve is opened during the induction stroke, to draw in fresh air that mixes with the trapped exhaust from the previous engine cycle to form a homogeneous mixture. This mixture is then compressed once the intake valve is closed, during the upward stroke of the piston. The compression culminates in a fast, uniform combustion process close to the top dead center position of the piston. Subsequent to this useful work is extracted from the engine as the piston moves down. Close to bottom dead center, the exhaust valve is opened, and a portion of the products of combustion is pushed out into the exhaust manifold during the upward stroke of the piston. The exhaust valve, however, is closed early enough to trap a significant amount of the combustion products in the cylinder, which is then recompressed as the piston reaches top dead center. Somewhere during this recompression stroke the fuel is injected into the cylinder.

Based on the above description, an HCCI engine cycle can be broken down into six well defined stages. This is done on the basis of several thermodynamic assumptions. Fresh charge induction is assumed to be adiabatic, and at a constant pressure. The compression, expansion and exhaust processes are modeled as isentropic processes. The combustion event itself, on account of the rapid nature of HCCI combustion, is assumed to be a constant volume (instantaneous) event.

With these assumptions, an HCCI cycle is modeled through the following six stages.

1. *Adiabatic induction at atmospheric pressure* culminating in *instantaneous mixing* of fuel, air and trapped exhaust at IVC
2. *Isentropic compression* from IVC to point of combustion
3. *Isochoric combustion* occurring instantaneously and uniformly
4. *Isentropic expansion* from point of instantaneous combustion to EVO
5. *Isentropic exhaust* from EVO to EVC
6. *Recompression* of trapped exhaust from EVC till IVO in the next cycle

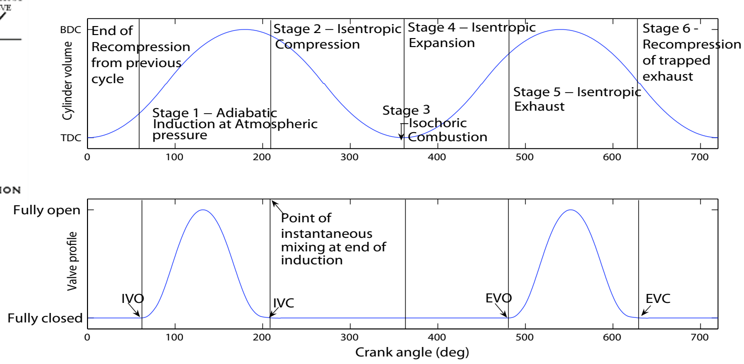

Figure 2. Stages in the HCCI cycle

Figure 2 shows these discrete stages with respect to the cylinder volume at any given position of the crank. The figure also shows typical valve profiles for the intake and exhaust valves.

Definition of inputs and outputs

The inputs to the system in the model are assumed to be the following:

1. *Moles of fuel injected* in the current cycle, $n_{f,k}$
2. *Volume at intake valve closure*, or the point at which instantaneous mixing between air, fuel and trapped exhaust is assumed to occur, $V_{IVC,k}$
3. *Volume at exhaust valve closure*, or the point at which the states of the system are determined, $V_{EVC,k}$ and
4. *Fraction of external EGR*, ψ_k. This assumes the presence, in addition to exhaust retention, of an external EGR mechanism where some portion of exhaust is routed from the exhaust manifold into the main incoming air stream. Though the amount of EGR itself is not easily measureable, the purpose of including it in the model is to determine the effect of EGR as an input on HCCI dynamics. An additional model to determine EGR amount can easily be added to the existing model.

The valve timings can be used to vary the relative amounts of air and trapped residual. A direct-inject system gives independent control of the amount of fuel in the cylinder, and is therefore a useful control knob.

In terms of the outputs of the model, what is ultimately desired is that the engine produce the amount of work required, and that combustion occur at the desired phasing. The outputs of the model are therefore chosen as quantities that are representative of these values, but are also easily measurable on an actual engine test-bed. These are

1. *Peak pressure*, $P_{3,k}$, which serves as a proxy for the net work output of the engine

2. *Angle of peak pressure*, $\theta_{23,k}$, which represents the phasing of the combustion event

Definition of states

In order to describe the dynamics of the HCCI process based on the framework laid down above, the *states* of the system need to be defined. The key thrust of this modeling work is to determine states for the HCCI process that

1. Represent a complete set of variables sufficient to describe the system dynamics to the desired level of detail for control
2. Have a physical/thermodynamic basis, ie, represent physical characteristics of the system that, at the most fundamental level, determine the nature of combustion in the engine

To this end, it would be of use to briefly examine combustion at the molecular level. The process of combustion is essentially dictated by two characteristics of the reactant mixture:

1. *Concentrations of the reactants*, which determines whether the reactant molecules are close enough to have sufficient collisions
2. *Temperature of the mixture*, which determines whether the collisions are energetic enough to cause a reaction

Choosing a set of state variables, therefore, that in some way represent these quantities, would give a fundamental basis for an HCCI model.

With specific reference to residual-affected HCCI, it is also important to recognize the pivotal role played by the trapped exhaust. It is the exhaust retained from the previous engine cycle that is used to heat (and dilute) the fresh charge for the current cycle, and is what induces the cycle-to-cycle coupling. This trapped exhaust, therefore, is essentially what carries information about combustion in one engine cycle through to the next.

Based on this, the states of the HCCI system can be chosen as those variables that capture the temperature and amounts of reactants in the trapped exhaust. Of the two reactants (fuel and O_2), the fuel is an input to the system, and is directly controlled through the fuel injector. Therefore the states are chosen as:

1. Moles of oxygen in the products of combustion at EVC, $n_{O_2,k}$
2. Temperature of the trapped exhaust at EVC, $T_{e,k}$

The subscript k here denotes the k'th engine cycle, where an engine cycle is assumed to start at EVC (end of exhaust, beginning of recompression). Using these state definitions, the various stages in an HCCI cycle can now be described.

Recompression Gasoline is assumed to have the formula C_7H_{13}. The stoichiometric combustion reaction can then be written as

$$C_7H_{13} + 10.25O_2 + 38.54N_2 \rightarrow 7CO_2 + 6.5H_2O + 38.54N_2 \quad (1)$$

If, instead of a stoichiometric mixture, we have n_f moles of fuel and n_a moles of air, the reaction then is (assuming lean combustion, which is typical in HCCI)

$$\begin{aligned} n_f C_7H_{13} + n_a(O_2 + 3.76N_2) \rightarrow 7n_f CO_2 + 6.5n_f H_2O \\ +(n_a - 10.25n_f)O_2 + 3.76n_a N_2 \end{aligned} \quad (2)$$

The fuel is injected into the cylinder at some point during recompression. The temperature of this fuel is assumed to be constant. Let the total moles of fuel injected into the cylinder be n_f. This is of course directly related to the duration of injection. The fuel, once injected into the cylinder, vaporizes, and so removes an amount of energy equal to $n_f h_{fg}$ from the cylinder, where h_{fg} is the heat of vaporization of gasoline.

At the end of the exhaust process in the previous cycle, a certain portion of the exhaust is trapped inside the cylinder by an early closing of the exhaust valve. Let total moles of exhaust in the cylinder at the point of EVC be n_e. Then by ideal gas law

$$n_e = \frac{P_{atm}V_{EVC}}{R_u T_e} \quad (3)$$

where the cylinder pressure at the end of exhaust is assumed to be atmospheric. Therefore, at this stage, we know the total moles of trapped exhaust as well as moles of oxygen (n_{O_2})in the cylinder, and temperature of the entire mixture (T_e) as these are the state variables. Individual concentrations of other constituents are unknown. It is, however, sufficient to know just total moles in the cylinder if we use bulk properties for the mixture, as opposed individual species properties in the thermodynamic calculations. This is a reasonable approximation because thermodynamic properties (such as specific heats) are similar for O_2, CO_2, H_2O, N_2 in the temperature ranges that are relevant [12].

During the recompression process, there is no inflow/outflow of species as the valves are closed. However, some heat transfer occurs, due to which temperature at the end of recompression is lower than at the beginning. The heat transfer during recompression and fresh charge induction can be modeled by relating temperature of trapped exhaust at the end of recompression and induction to the temperature at EVC by a simple zero-dimensional heat loss model.

$$T_{1,exh} = \chi T_{e,k} \quad (4)$$

where χ is a constant factor determined empirically and $T_{e,k}$ is one of the states.

Adiabatic induction followed by instantaneous mixing Fresh air is inducted into the cylinder from IVO to IVC at a constant pressure (assumed to be atmospheric) and temperature. This is then assumed to mix instantaneously at IVC with the trapped exhaust and fuel. To obtain the state of the components of the cylinder after mixing, we apply the first law of thermodynamics. A constant average specific heat for the entire mixture is used. We assume that $n_{a,k}$ moles of air and $\psi_k n_{a,k}$ moles of cold external EGR gas enter the cylinder together at a fixed temperature T_i. Total moles inside the cylinder (neglecting quantity of fuel), is then given by $n_{tot,k} = n_{a,k}(1+\psi_k) + n_{e,k}$.

Applying the 1st law to the mixing process based on the above assumptions

$$\bar{C_p}\left\{n_{a,k}(1+\psi_k)T_i + \chi n_{e,k}T_{e,k}\right\} - n_{f,k}h_{fg} = \bar{C_p}\left\{n_{a,k}(1+\psi_k) + n_{e,k}\right\}T_{1,k} \quad (5)$$

Here it is assumed that a part of the sensible energy is removed from the system due to vaporization of the fuel.

Rearranging equation 5,

$$T_{1,k} = \frac{n_{a,k}(1+\psi_k)T_i + \chi n_{e,k}T_{e,k} - C_1 n_{f,k}}{n_{a,k}(1+\psi_k) + n_{e,k}} \quad (6)$$

where $C_1 = h_{fg}/\bar{C_p}$

Such a formulation also gives a very simple expression for the moles of air entering the cylinder during the current cycle. Applying the ideal gas law (and neglecting moles of fuel inside the cylinder),

$$n_{a,k}(1+\psi_k) + n_{e,k} = \frac{P_{i,k}V_{IVC,k}}{R_u T_{1,k}} \quad (7)$$

Substituting for $T_{1,k}$ from (6) and for $n_{e,k}$ from (3) and rearranging

$$n_{a,k} = \frac{P_{i,k}V_{IVC,k} + R_u C_1 n_{f,k} - \chi P_{atm}V_{EVC,k}}{R_u T_i(1+\psi_k)} \quad (8)$$

Total moles of oxygen now present in the cylinder (after induction) is given by

$$n_{O_2,1} = 0.21 n_{a,k} + n_{O_2,k}\left(1 + \frac{\psi_k n_{a,k}}{n_{e,k}}\right) \quad (9)$$

where $\frac{n_{O_2,k}\psi_k n_{a,k}}{n_{e,k}}$ represents amount of oxygen in $\psi_k n_{a,k}$ moles of external EGR, given that $n_{e,k}$ moles of exhaust contains $n_{O_2,k}$ moles of oxygen.

Using the ideal gas law and (8) an expression for $T_{1,k}$ is obtained in terms of the state variables

$$T_{1,k} = \frac{P_{i,k}V_{IVC,k}}{R_u\left\{n_{a,k}(1+\psi_k) + n_{e,k}\right\}} \quad (10)$$

Pressure and volume at this point are given by $P_{1,k} = P_{i,k}$ and $V_{1,k} = V_{IVC,k}$. Therefore the state of the mixture at the start of compression is completely known.

Isentropic compression Isentropic compression is assumed, and therefore

$$T_{2,k} = \left(\frac{V_{IVC,k}}{V_{23,k}}\right)^{\gamma-1} T_{1,k} \quad (11)$$

$$P_{2,k} = \left(\frac{V_{IVC,k}}{V_{23,k}}\right)^{\gamma} P_{i,k} \quad (12)$$

Here the term $V_{23,k}$ represents the volume of the cylinder at the point where instantaneous combustion is assumed to occur. A model for determining the instant of combustion is presented subsequently.

Isochoric combustion HCCI combustion is typically very fast, and therefore an instantaneous, constant volume combustion can be assumed to occur. From (2) and (9), the combustion equation in terms of just the reacting species can be written as

$$n_{f,k}C_7H_{13} + \left\{0.21 n_{a,k} + n_{O_2,k}\left(1 + \frac{\psi_k n_{a,k}}{n_{e,k}}\right)\right\}O_2 \rightarrow 7n_{f,k}CO_2 + 6.5n_{f,k}H_2O + \left\{0.21 n_{a,k} - 10.25 n_{f,k} + n_{O_2,k}\left(1 + \frac{\psi_k n_{a,k}}{n_{e,k}}\right)\right\}O_2 \quad (13)$$

Applying the first law to the combustion reaction

$$m\frac{du}{dt} = \dot{Q}_{comb} - \dot{W} \quad (14)$$

As the combustion is assumed to occur at constant volume, the piston work, $\dot{W} = p\dot{V}$, is zero. The first law then becomes:

$$m\frac{du}{dt} = \dot{Q}_{comb} \quad (15)$$

Integrating this expression yields

$$U_2 = U_3 + Q_{comb} \quad (16)$$

The heat loss during the entire HCCI cycle can be taken as a fraction of the fuel heating value. The first law then becomes (assuming positive lower heating value for fuel)

$$U_2 = U_3 - (1-\varepsilon) n_{f,k} LHV_f \tag{17}$$

Again, assuming that all constituents (except the fuel) have the same specific heat, and substituting for U_2 and U_3

$$\begin{aligned}&\left\{\bar{C}_{v,f} n_{f,k} + \bar{C}_v \left(n_{a,k}(1+\psi_k) + n_{e,k}\right)\right\}(T_{2,k} - T_{ref})\\ &= \bar{C}_v \left\{3.25 n_{f,k} + n_{a,k}(1+\psi_k) + n_{e,k}\right\}(T_{3,k} - T_{ref})\\ &\quad - (1-\varepsilon) n_{f,k} LHV_f\end{aligned} \tag{18}$$

Rearranging,

$$T_{3,k} = \frac{C_2 n_{f,k} + \left\{\bar{C}_{v,f} n_{f,k} + \bar{C}_v \left(n_{a,k}(1+\psi_k) + n_{e,k}\right)\right\} T_{2,k}}{\bar{C}_v \left\{3.25 n_{f,k} + n_{a,k}(1+\psi_k) + n_{e,k}\right\}} \tag{19}$$

where $C_2 = (1-\varepsilon)LHV_f + (3.25\bar{C}_v - \bar{C}_{v,f})T_{ref}$

Applying the ideal gas law before and after combustion,

$$\begin{aligned}N_2 &= \frac{P_2 V_{23}}{R_u T_2}\\ N_3 &= \frac{P_3 V_{23}}{R_u T_3}\end{aligned} \tag{20}$$

From inspection of the combustion reaction it is easy to see that $\frac{N_3}{N_2} \approx 1$. Therefore

$$P_{3,k} = P_{2,k} \frac{T_{3,k}}{T_{2,k}} \tag{21}$$

Rearranging (19)

$$T_{2,k} = \frac{\bar{C}_v \left\{3.25 n_{f,k} + n_{a,k}(1+\psi_k) + n_{e,k}\right\} T_{3,k} - C_2 n_{f,k}}{\left\{\bar{C}_{v,f} n_{f,k} + \bar{C}_v \left(n_{a,k}(1+\psi_k) + n_{e,k}\right)\right\}} \tag{22}$$

Substituting (22) and (12) in (21)

$$\begin{aligned}P_{3,k} &= \left(\frac{V_{IVC,k}}{V_{23,k}}\right)^{\gamma} *\\ &\frac{\left\{\bar{C}_{v,f} n_{f,k} + \bar{C}_v \left(n_{a,k}(1+\psi_k) + n_{e,k}\right)\right\} P_{i,k} T_{3,k}}{\bar{C}_v \left\{3.25 n_{f,k} + n_{a,k}(1+\psi_k) + n_{e,k}\right\} T_{3,k} - C_2 n_{f,k}}\end{aligned} \tag{23}$$

Isentropic expansion Isentropic expansion is assumed till the opening of the exhaust valve, and so

$$T_{4,k} = \left(\frac{V_{23,k}}{V_{4,k}}\right)^{\gamma-1} T_{3,k} \tag{24}$$

$$P_{4,k} = \left(\frac{V_{23,k}}{V_{4,k}}\right)^{\gamma} P_{3,k} \tag{25}$$

Isentropic exhaust The exhaust process is also modeled as an isentropic process, assuming that the exhaust manifold is at atmospheric pressure.

$$\begin{aligned}T_{5,k} &= \left(\frac{P_{atm}}{P_{4,k}}\right)^{\frac{\gamma-1}{\gamma}} T_{4,k}\\ &= \left(\frac{P_{atm}}{P_{3,k}}\right)^{\frac{\gamma-1}{\gamma}} T_{3,k}\end{aligned} \tag{26}$$

Applying the ideal gas law at the beginning and end of the exhaust process, the number of moles of products in the cylinder before and after exhaust are obtained, the ratio of which gives an expression for the fraction of trapped exhaust, β

$$\begin{aligned}\beta &= \frac{N_5}{N_4} = \frac{V_5 P_5 T_4}{V_4 P_4 T_5}\\ &= \left(\frac{P_{atm}}{P_3}\right)^{\frac{1}{\gamma}} \frac{V_5}{V_{23}}\end{aligned} \tag{27}$$

From (13) and (27), the state update equation for $n_{O_2,k}$ is obtained.

$$n_{O_2,k+1} = \beta_k \left\{0.21 n_{a,k} - 10.25 n_{f,k} + n_{O_2,k}\left(1 + \frac{\psi_k n_{a,k}}{n_{e,k}}\right)\right\} \tag{28}$$

Simplifications

To obtain an expression for the peak pressure ($P_{3,k}$) in terms of the states and inputs, we need to substitute for $T_{3,k}$ in (23). A simplification can be made here, by comparing the denominator in (22) with the first term in the denominator of (23), and recognizing that $n_{f,k} \ll n_{a,k}$. We can then assume

$$\begin{aligned}A_k &= \bar{C}_v \left\{3.25 n_{f,k} + n_{a,k}(1+\psi_k) + n_{e,k}\right\}\\ &\approx \left\{\bar{C}_{v,f} n_{f,k} + \bar{C}_v \left(n_{a,k}(1+\psi_k) + n_{e,k}\right)\right\}\end{aligned} \tag{29}$$

Substituting (29) in (19) and (23)

$$T_{3,k} \approx \frac{C_2 n_{f,k} + A_k T_{2,k}}{A_k} \tag{30}$$

and

$$P_{3,k} = \left(\frac{V_{IVC,k}}{V_{23,k}}\right)^{\gamma} \frac{A_k P_{i,k} T_{3,k}}{A_k T_{3,k} - C_2 n_{f,k}} \tag{31}$$

Substituting for $T_{3,k}$ in (31) and rearranging, an expression for the output $P_{3,k}$ in terms of the states and inputs is obtained

$$P_{3,k} = \frac{C_2 n_{f,k} \left\{ P_i V_{IVC,k} T_{e,k} + R_u C_1 n_{f,k} T_{e,k} - P_{atm} V_{EVC,k} (\chi T_{e,k} - T_i) \right\}}{A V_{23,k} T_i T_{e,k}} + \frac{\left(\frac{V_{IVC,k}}{V_{23,k}}\right)^{\gamma-1} P_{i,k} V_{IVC,k}}{V_{23,k}} \tag{32}$$

This gives one output equation in the state space form of the model.

The temperature of trapped exhaust at EVC is then equal to T_5

$$T_{e,k+1} = T_{5,k} = \left(\frac{P_{atm}}{P_{3,k}}\right)^{\frac{\gamma-1}{\gamma}} T_{3,k} \tag{33}$$

Substituting from (32) we get the state update equation for T_e, shown in (34) on top of the next page This is the second state update equation.

Combustion phasing modeling

In order to develop a model to determine the phasing of combustion, a simple global Arrhenius rate model is used, which has been shown to be adequate to capture the dynamics affecting phasing ([6], [7]). The reaction rate for the overall combustion reaction is given as

$$RR = A_{th} e^{\left(\frac{E_a}{R_u T}\right)} [C_7H_{13}]^a [O_2]^b \tag{35}$$

where E_a is the activation energy and A_{th} is a pre-exponential factor. Integrating this global Arrhenius rate equation from IVC to the point of combustion gives an expression of the form

$$\int RR = \int_{\theta_{IVC}}^{\theta_{th}} A_{th} e^{\left(\frac{E_a}{R_u T}\right)} [C_7H_{13}]^a [O_2]^b dt \tag{36}$$

Combustion can then be modeled to begin when this integral crosses a certain threshold value, K_{th}. The point at which the peak in-cylinder pressure is reached, θ_{23} is related to the point at which the threshold is crossed as $\theta_{th} = \theta_{23} - \delta\theta$, where $\delta\theta$ is assumed to be constant as a consequence of approximating the combustion event to be a function of the crank angle.

The integration can be simplified by approximating the integrand by its value at TDC, and beginning integration at this point, a justifiable assumption as the value of the integrand is largest at TDC. In this case a linear expression for the phasing θ_{23} is obtained in terms of the Arrhenius threshold.

$$\begin{aligned} \hat{K}_{th} &= \int_{\theta_{IVC}}^{\theta_{23}-\delta\theta} A_{th} e^{\left(\frac{E_a}{R_u T_{TDC}}\right)} [C_7H_{13}]^a_{TDC} [O_2]^b_{TDC} d\theta / \omega_k \\ &\approx A_{th} e^{\frac{-E_a}{R_u T_{TDC}}} [C_7H_{13}]^a_{TDC} [O_2]^b_{TDC} \frac{(\theta_{23} - \theta_{TDC} - \delta\theta)}{\omega_k} \end{aligned} \tag{37}$$

where ω_k is the engine speed.

Here

$$\begin{aligned} T_{TDC} &= \left(\frac{V_{IVC,k}}{V_{TDC}}\right)^{\gamma-1} T_{1,k} \\ [C_7H_{13}]_{TDC} &= \frac{n_{f,k}}{V_{TDC}} \\ [O_2]_{TDC} &= \frac{0.21 n_{a,k} + \left(1 + \frac{\psi_k n_{a,k}}{n_{e,k}}\right) n_{O_2,k}}{V_{TDC}} \end{aligned} \tag{38}$$

Substituting (38) and (10) in (37) and rearranging, an expression for the combustion phasing is obtained, shown in (39) on top of the next page. This is the second output equation in the state space form of the model. With this, there is now a closed form solution for the outputs in terms of the states and inputs, and the time-update equations for the states.

The cylinder volume at the point of combustion can be obtained using the simple volume equation for the cylinder as a function of the crank position as given in [13].

$$V(\theta) = V_c + \frac{\pi B_{cyl}^2}{4} \left(L_{cyl} + a_{cyl}(1 - cos\theta) - \sqrt{L_{cyl}^2 - a_{cyl}^2 \sin^2\theta} \right) \tag{40}$$

Model Summary

A two state model of the HCCI process is obtained in the following nonlinear state-space form

$$\begin{aligned} x_{k+1} &= F(x_k, u_k) \\ y_k &= G(x_k, u_k) \end{aligned} \tag{41}$$

The states, inputs and outputs are given by

$$x_k = \begin{bmatrix} n_{O_2,k} \\ \tilde{T}_{e,k} \end{bmatrix}, u_k = \begin{bmatrix} n_{f,k} \\ V_{IVC,k} \\ V_{EVC,k} \\ \psi_k \end{bmatrix}, y_k = \begin{bmatrix} P_{pk,k} \\ \theta_{pk,k} \end{bmatrix} \tag{42}$$

$$T_{e,k+1} = \frac{(P_{atm}V_{23,k}T_iT_{e,k})^{\frac{\gamma-1}{\gamma}}}{A_k^{\frac{1}{\gamma}}\left\{P_iV_{IVC,k}T_{e,k}+R_uC_1n_{f,k}T_{e,k}-P_{atm}V_{EVC,k}(\chi T_{e,k}-T_i)\right\}}\left[A_k\left(\frac{V_{IVC,k}}{V_{23,k}}\right)^{\gamma-1}P_{i,k}V_{IVC,k}T_iT_{e,k}+C_2n_{f,k}\left\{P_iV_{IVC,k}T_{e,k}+R_uC_1n_{f,k}T_{e,k}-P_{atm}V_{EVC,k}(\chi T_{e,k}-T_i)\right\}\right]^{\frac{1}{\gamma}} \tag{34}$$

$$\theta_{23,k} = \frac{\dfrac{K_{th}(V_{TDC})^{a+b}\omega_k}{A_{th}(n_{f,k})^a\left\{0.21n_{a,k}+\left(1+\frac{\psi_k n_{a,k}}{n_{e,k}}\right)n_{O_2,k}\right\}^b}}{exp\left[\frac{-E_a}{R_u}\left(\frac{V_{TDC}}{V_{IVC,k}}\right)^{\gamma-1}\left\{\frac{P_iV_{IVC,k}T_{e,k}+R_uC_1n_{f,k}T_{e,k}-P_{atm}V_{EVC,k}(\chi T_{e,k}-T_i)}{P_iV_{IVC,k}T_iT_{e,k}}\right\}\right]}+\theta_{TDC}+\delta\theta \tag{39}$$

Table 1. Engine parameters

Parameter	Value	Units
Engine speed	1000	rpm
Stroke	94.6	mm
Connecting rod length	152.2	mm
Bore diameter	86	mm
Compression ratio	12	

The two state update equations are given in (28) and (34), and the two output equations are given in (32) and (39).

MODEL VALIDATION IN SIMULATION

The control model described above was validated in simulation against a more complete model of HCCI combustion developed previously [6,7]. This is a continuous time, ten-state model that includes much of the complex thermodynamics of the HCCI process. Valve flows are modeled using compressible flow equations, heat transfer occurs continuously throughout the engine cycle and is modeled by the extended Woschni correlation [14], and the combustion event is of finite duration, and is captured by a Wiebe function. It is however too complex for controller development and real-time implementation.

To compare the two models, the properties of the cylinder contents at the end of each of the stages in the HCCI cycle are obtained at a particular steady-state operating condition. Of specific importance are the pressure and temperature in the cylinder at each of these locations and the location of peak pressure. These quantities are compared across the models.

Engine parameters and particular operating condition characteristics used in simulation are shown in Tables 1 and 2 respectively. The particular operating condition simulated has been chosen arbitrarily as one of the test cases for which the complex simulation model was parametrized based on experiments. Figures 3 and 4 show the evolution of in-cylinder pressure and temperature respectively during one HCCI cycle as predicted by

Table 2. Operating point at which continuous simulation and simple control model are compared

Parameter	Value	Units
IVO	75	CAD
IVC	195	CAD
EVO	525	CAD
EVC	645	CAD
Mass of fuel injected per cycle	8	mg
Peak pressure	4350	kPa
Angle of Peak Pressure	365	CAD

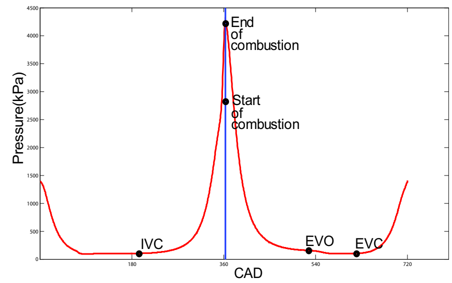

Figure 3. Comparison of Control model and Continuous time simulation - In-Cylinder Pressure

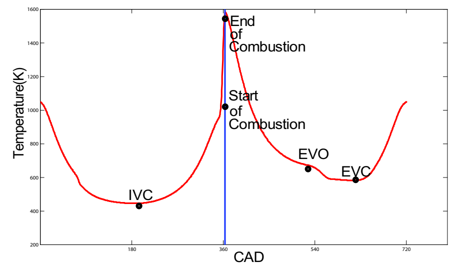

Figure 4. Comparison of Control model and Continuous time simulation - In-Cylinder Temperature

the continuous time simulation. Values obtained from the simpler control model at several discrete points are indicated on the plots. As seen, the control model accurately predicts

1. Peak pressure in the cycle
2. Crank angle at which peak pressure occurs in the cycle
3. Temperature of trapped exhaust at EVC
4. Temperatures and pressures at other points in the cycle

There is a loss of accuracy in intra-cycle dynamics in the two state model as compared to the continuous time ten state model. However the cycle to cycle dynamics are captured accurately enough to be suitable for control. Earlier work [10, 11] has shown that two states are sufficient to model the cycle to cycle dynamics of HCCI and have been used to control the process dynamically.

LINEARIZATION

In order to demonstrate the value of this model as a platform for controller synthesis, a simple controller is now designed based on the model. It is first linearized about an operating point, so as to allow the synthesis of linear controllers. Linear expressions are taken for any quantity a_k of the form $a_k = \bar{a}_k + \hat{a}_k$. Here $\bar{a}_k$ represents the value of the quantity a at the nominal operating condition, and $\hat{a}_k$ represents its deviation from that operating point. These expressions are then substituted in the nonlinear state and output update equations, and Taylor expansions to the first term give linear system equations around the particular operating condition.

$$\begin{aligned} \hat{x}_{k+1} &= A\hat{x}_k + B\hat{u}_k \\ \hat{y}_k &= C\hat{x}_k + D\hat{u}_k \end{aligned} \tag{43}$$

where A, B, C and D are matrices. As the linearization is performed analytically, this gives the form of a general linear model. Expressions for the matrices are functions of the operating point at which the system is linearized, engine parameters, and physical properties of the cylinder constituents. Substituting these in, values for the matrices can be obtained at any operating condition.

CONTROLLER SYNTHESIS AND IMPLEMENTATION

As an example of the applicability of this model, we now demonstrate the synthesis of an HCCI controller based on the model. Using engine parameters, and properties of fuel and air (obtained from [13]), the values of the matrices for the linearized system at an operating point (described in Table 2) are determined. This gives a linear model for the system at that point, using which a variety of simple closed-loop controllers can be synthesized. Here a simple LQR controller assuming full state

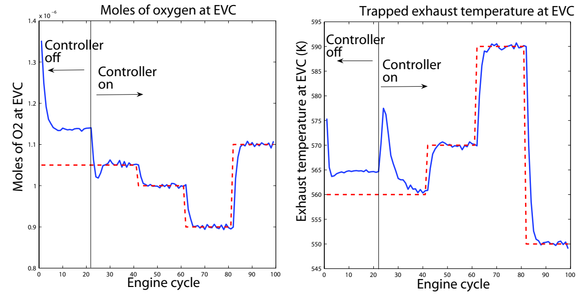

Figure 5. LQR controller implemented in simulation - evolution of states Dashed line - Desired trajectory, Solid line - Actual trajectory

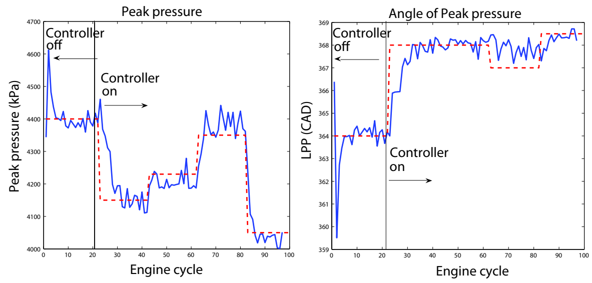

Figure 6. LQR controller implemented in simulation - evolution of outputs Dashed line - Outputs corresponding to desired state trajectory, Solid line - Actual output trajectory

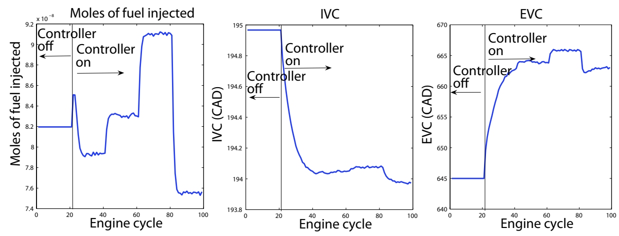

Figure 7. LQR controller implemented in simulation - inputs commanded

feedback has been derived to track a desired state trajectory. This controller is of the form

$$\hat{u}_k = -K_{lqr}\hat{x}_k \tag{44}$$

and minimizes the cost function

$$J = \Sigma(\hat{x}_k Q\hat{x}_k + \hat{u}_k R\hat{u}_k) \tag{45}$$

This controller is implemented on the continuous time simulation model. The R matrix is chosen so as to have a very large cost on the EGR input (ψ) - and so effectively the main inputs used are V_{IVC}, V_{EVC} and n_f.

As shown in Figure 5, the controller is used to track a desired state trajectory (shown by dashed line). The controller is first switched on after 20 engine cycles, after which the system states are seen to track the desired trajectory very closely. Response time is fairly quick, and is of the order of 5-6 engine cycles. Figure 6 shows the behavior of the model outputs (peak pressure and angle of peak pressure) as the system tracks this desired state trajectory. The inputs commanded by the LQR controller are shown in Figure 7.

CONCLUSIONS

HCCI, with the benefits it offers, presents one of the most promising solutions to today's energy and ecological problems. However the challenges with achieving and maintaining HCCI in an engine necessitate the synthesis of a closed-loop control strategy for the HCCI process. The first step towards the development of such a strategy is the design of a model of the HCCI process. One possible approach to this end has been described in this paper. The two state model presented here was aimed at capturing the behavior of HCCI based on the underlying thermodynamics of the process. The model states were selected so as to represent mixture temperature and reactant concentrations, which are the key determinants of the nature of HCCI combustion. In addition, the trapped exhaust from one cycle represents the fundamental agent of information transfer to the next cycle - and therefore the states for the model were chosen as moles of oxygen in, and temperature of, the trapped exhaust at EVC. With this set of states, a nonlinear model of HCCI was obtained. This model effectively maps the engine thermodynamics to a control-oriented state-space description of HCCI. As a physically motivated control model, therefore, it represents an ideal foundation for the synthesis of a variety of model-based control strategies. As an example, an LQR controller has been demonstrated in simulation and used to track a desired system trajectory.

FUTURE WORK

The states of the model as formulated are not directly measurable on an engine, and the final objective is control of desired output trajectories. Therefore the next step is to develop an observer that can be used to estimate the states. The state estimate can then used to track a desired output trajectory.

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