MODELING CYCLE-TO-CYCLE COUPLING IN HCCI ENGINES UTILIZING VARIABLE VALVE ACTUATION

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Abstract: In order to capture the effect of cycle-to-cycle coupling that is inherent in residual-affected homogeneous charge compression ignition (HCCI) engines, a simple, control-oriented, single-zone model of HCCI combustion is presented. The inclusion of an exhaust manifold model ties the exhausted gas from one cycle to that re-inducted on the next cycle. Multi-cycle simulations are completed and shown to have the same general steady state and transient characteristics as an experimental system. Predicted combustion phasing and in-cylinder pressure values agree very well with experiment.

Keywords: internal combustion engines, control oriented models, engine modeling, model-based control, automotive emissions, engine efficiency

1. INTRODUCTION

Homogeneous charge compression ignition (HCCI) holds great promise as a means to reduce NO_x emissions and increase efficiency in internal combustion engines (Caton *et al.*, 2003). HCCI is achieved by uniform auto-ignition of a homogeneous mixture of combustion gases. This leads to a low post-combustion temperature, which significantly reduces NO_x emissions. There are several methods used to initiate HCCI, such as heating or pre-compressing the intake air (Tunestal *et al.*, 2001; Martinez-Frias *et al.*, 2000), trapping exhaust gases from the previous cycle by closing the exhaust valve early (Law *et al.*, 2001), modulating intake and exhaust flows using variable valve actuation (VVA) to re-induct exhaust from the previous cycle (Caton *et al.*, 2003; Law *et al.*, 2001) or some combination of these (Agrell *et al.*, 2003; Hyvönen *et al.*, 2003).

Regardless of the method chosen, however, HCCI combustion exhibits some fundamental control challenges with regards to combustion phasing and work output. Unlike spark ignition (SI) or diesel engines, where the combustion is initiated via spark and fuel injection, respectively, HCCI has no specific event that initiates combustion. Additionally, for residual-affected HCCI achieved with VVA, there is cycle-to-cycle coupling that must also be considered since products from the previous cycle are either re-inducted or trapped. Ensuring that combustion occurs with acceptable timing, or at all, is more complicated than in the case of either SI or diesel combustion. Combustion phasing in HCCI is dominated by chemical kinetics, which depends on the in-cylinder concentrations of reactants and products, their temperature and when they are allowed to begin mixing. Work output is dependent on both the combustion phasing and the amount of reactant species present in the cylinder. Thus to control HCCI through VVA it is essential to understand how the valves influence mass flows and combustion phasing. Additionally, it is important to know how previous combustion cycles influence the temperature of the reinducted products.

Various models of HCCI combustion with more complexity than that presented here have been developed. These include multi-zone models (Ogink and

Golovitchev, 2002; Fiveland and Assanis, 2002) and multi-dimensional CFD models (Kong *et al.*, 2001). While these approaches can be expected to more accurately predict the performance and emissions in HCCI combustion, this work shows that simple models can accurately capture combustion phasing, cycle-to-cycle coupling, and work output.

In order to understand the effect of the VVA system on HCCI combustion, a single-zone model of a single cylinder engine outfitted with VVA has been introduced in previous work (Shaver *et al.*, 2003). To capture the combustion phasing in a simple and intuitive way, an integrated Arrhenius rate expression is used. This relation relates the in-cylinder temperature, reactant concentrations and the amount of time available for reactant-product mixing (dictated by the intake valve opening (IVO) time) to the crank angle position where combustion is initiated. An exhaust manifold model to capture cycle-to-cycle coupling through the product gases has been added to the modeling completed in the previous work. Steady-state and transient simulation results demonstrate that simple models can indeed capture combustion phasing, load, and cycle-to-cycle interaction for HCCI engines with VVA.

2. MODELING APPROACH

The modeling is based on an open system first law analysis. Steady state compressible flow relations are used to model the mass flow through the intake and exhaust valves. The model includes nine states: the cylinder volume, V; the temperature, T; the concentrations of propane, [C_3H_8], oxygen, [O_2], nitrogen, [N_2], carbon dioxide, [C_2O], water, [H_2O]; the mass in the exhaust manifold, m_e; and the internal energy of the product gases in the exhaust, u_e.

2.1 Volume Rate Equation

The in-cylinder volume and its derivative are given by the following well-known slider-crank formula:

$$\dot{V} = \frac{\pi}{4} B^2 a \dot{\theta} sin\theta \left(1 + a \frac{cos\theta}{\sqrt{(L^2 - a^2 sin^2\theta)}} \right) \qquad (1)$$

where $\omega = \dot{\theta}$ is the rotational speed of the crankshaft, a is half of the stroke length, L is the connecting rod length, B is the bore diameter and V_c is the clearance volume at top dead center.

2.2 Valve Flow Equations

The mass flow through the valves consists of flow from intake manifold to cylinder, $\dot{m}_{ic}$, from cylinder to exhaust manifold, $\dot{m}_{ce}$, and from exhaust manifold to cylinder, $\dot{m}_{ec}$, as shown in Figure 1. Figure 1 also shows the general shape of the valve lift profiles used. It is the intake valve opening (IVO) and exhaust valve closing (EVC) timings that are varied for different operating conditions in this study, while the intake valve closing (IVC) and exhaust valve opening (EVO) timings are held constant at 220 and 490 degrees, respectively. Equations for the mass flow rates are

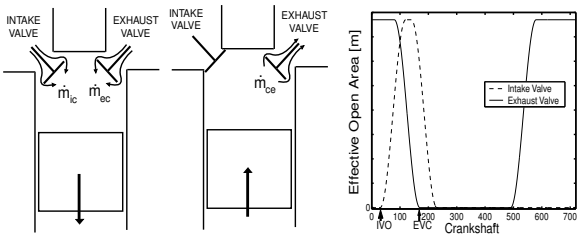

Fig. 1. Valve Mass Flows: left - induction flows with intake and exhaust valves open, center - exhaust flow, right - valve timings

developed using a compressible, steady state, one-dimensional, isentropic flow analysis for a restriction, where real gas flow effects are included by means of a discharge coefficient, C_D. The relations for the mass flows are:

$$\dot{m} = \frac{C_D A_R p_o}{\sqrt{RT_o}} \left(\frac{p_T}{p_o} \right)^{1/\gamma} \left[\frac{2\gamma}{\gamma - 1} \left[1 - \left(\frac{p_T}{p_o} \right)^{(\gamma-1)/\gamma} \right] \right]^{1/2} \qquad (2)$$

for unchoked flow ($p_T/p_o > [2/(\gamma+1)]^{\gamma/(\gamma-1)}$), and:

$$\dot{m} = \frac{C_D A_R p_o}{\sqrt{RT_o}} \sqrt{\gamma} \left[\frac{2}{\gamma+1} \right]^{(\gamma+1)/2(\gamma-1)} \qquad (3)$$

for choked flow ($p_T/p_o \leq [2/(\gamma+1)]^{\gamma/(\gamma-1)}$), where A_R is the effective open area for the valve, p_o is the upstream stagnation pressure, T_o is the downstream stagnation temperature and p_T is the downstream stagnation pressure.

For the mass flow of the reactant gas into the cylinder through the intake valve, $\dot{m}_{ic}$, p_o is the intake manifold pressure, assumed to be atmospheric, and p_T is the cylinder pressure, p. For the mass flow of burnt products out of the cylinder through the exhaust valve, $\dot{m}_{ce}$, p_o is the cylinder pressure, p, and p_T is the exhaust manifold pressure, assumed to be atmospheric. For the reinducted exhaust from the previous cycle through the exhaust valve, $\dot{m}_{ec}$, p_o is the exhaust manifold pressure, and p_T is the cylinder pressure, p. Note that manifold pressure dynamics due to valve timing transients (Stefanopoulou, 2001) are not included, but could be implemented if desired. Additionally, note that it is assumed that there is no flow from cylinder to intake manifold. This is a reasonable assumption for the experimental system studied in this paper. However, allowing flow from cylinder to intake manifold would be simple to include in the model if necessary.

2.3 Concentration Rate Equations

The rate of change of concentration for species i, $[\dot{X}_i]$ is related to number of moles of species i in the cylinder, N_i, by:

$$[\dot{X}_i] = \frac{d}{dt}\left(\frac{N_i}{V}\right) = \frac{\dot{N}_i}{V} - \frac{\dot{V}N_i}{V^2} = w_i - \frac{\dot{V}N_i}{V^2} \quad (4)$$

where w_i, the rate of change of moles of species i per unit volume has been defined as:

$$w_i = \frac{\dot{N}_i}{V} \quad (5)$$

This value has two contributions: the rate of change of moles of species i per unit volume due to the combustion reactions, $w_{rxn,i}$, and due to flow through the valves under the control of the VVA system, $w_{valves,i}$, such that:

$$w_i = w_{rxn,i} + w_{valves,i} \quad (6)$$

The combustion reaction rate, $w_{rxn,i}$, is determined through the use of a combustion chemistry mechanism. The approach used is outlined in Section 2.5.

Given the mass flow rates ($\dot{m}_{ic,i}$, $\dot{m}_{ec,i}$ and $\dot{m}_{ce,i}$) from the analysis in Section 2.2, the rate of change of moles of species i per unit volume due to flow through the valves, $w_{valves,i}$, can be found using the species mass fractions:

$$w_{valves,i} = w_{ic,i} + w_{ec,i} - w_{ce,i} \quad (7)$$

where:

$$w_{ic,i} = \frac{Y_{i,i}\dot{m}_{ic}}{VMW_i} \quad (8)$$

$$w_{ec,i} = \frac{Y_{e,i}\dot{m}_{ec}}{VMW_i} \quad (9)$$

$$w_{ce,i} = \frac{Y_{c,i}\dot{m}_{ce}}{VMW_i} \quad (10)$$

Here $Y_{i,i}$, $Y_{e,i}$ and $Y_{c,i}$ are the mass fractions of species i in the inlet manifold, exhaust manifold and cylinder, respectively. It is assumed that a stoichiometric mixture is present in the intake manifold. Further, it is assumed that only the major combustion products of CO_2, H_2O and N_2 are re-inducted into the cylinder through the exhaust. Therefore $Y_{i,i}$ and $Y_{e,i}$ are constant. Note that other intake and exhaust manifold compositions can be considered, but in any case the manifold mass fractions are constant during an engine cycle. However, the mass fraction of species i in the cylinder, $Y_{c,i}$, is constantly changing, and can be related to the concentration states as:

$$Y_{c,i} = \frac{[X_i]MW_i}{\sum [X_i]MW_i} \quad (11)$$

2.4 Temperature Rate Equations

In order to derive a differential equation for the temperature of the gas inside the cylinder, the first law of thermodynamics for an open system and the ideal gas law are combined as outlined below. The first law of thermodynamics for the cylinder is:

$$\frac{d(m_c u_c)}{dt} = \dot{Q}_c - \dot{W}_c + \dot{m}_{ic}h_i + \dot{m}_{ec}h_e - \dot{m}_{ce}h_c \quad (12)$$

where m_c is the mass of species in the cylinder, u_c is the in-cylinder internal energy, $\dot{Q}_c = -\bar{h}_c A_s(T - T_{wall})$ is the in-cylinder heat transfer rate, $\dot{W}_c = p\dot{V}$ is the in-cylinder work, h_i is the enthalpy of species in the intake manifold, h_e is the enthalpy of species in the exhaust manifold, and h_c is the enthalpy of the species in the cylinder. Note that the convective heat transfer rate is modeled in the standard way, where $\bar{h}_c$ is the average convection coefficient, A_s is the in-cylinder surface area, and T_{wall} is the average cylinder wall temperature. The wall temperature is approximated as 400K, a common assumption (Stone, 1999). Using the definition of enthalpy, $h_c = u_c + pV/m_c$, Equation 12 can be re-written as:

$$\frac{d(m_c h_c)}{dt} = \dot{Q}_c + \dot{p}V + \dot{m_{ic}}h_i + \dot{m_{ec}}h_e - \dot{m_{ce}}h_c \quad (13)$$

Expanding the enthalpy to show the contributions of the species in the cylinder yields:

$$m_c h_c = H_c = \sum N_i \hat{h}_{c,i} \quad (14)$$

where N_i is the number of moles of species i in the cylinder, H is the total enthalpy of species in Joules in the cylinder, and $\hat{h}_{c,i}$ is the enthalpy of species i in the cylinder on a molar basis.

Noting that the rate of change of enthalpy per unit mole of species i can be represented as $\dot{\hat{h}}_{c,i} = c_{p,i}(T)\dot{T}$, where $c_{p,i}(T)$ is the specific heat of species i per mole at temperature T, Equations 14 and 4 can be combined to give:

$$\frac{d(m_c h_c)}{dt} = V\left(\sum [\dot{X}_i]\hat{h}_{c,i} + \dot{T}\sum [X_i]c_{p,i}(T)\right) + \dot{V}\sum [X_i]\hat{h}_{c,i} \quad (15)$$

In-cylinder pressure and its derivative can be related to the concentrations and temperature through the ideal gas law as:

$$p = \sum [X_i]RT \quad (16)$$

$$\dot{p} = \frac{p\sum [\dot{X}_i]}{\sum [X_i]} + \frac{p\dot{T}}{T} \quad (17)$$

The in-cylinder mass and its derivative may be related to the species concentrations, molecular weights and volume as:

$$m_c = V\sum [X_i]MW_i \quad (18)$$

$$\dot{m}_c = \dot{V}\sum [X_i]MW_i + V\sum [\dot{X}_i]MW_i \quad (19)$$

Equating the right sides of Equations 13 and 15, substituting Equations 17, 18, and 19, and rearranging yields a differential equation for temperature:

$$\dot{T} = \frac{\frac{\dot{Q}}{V} - (\sum[\dot{X}_i]\hat{h}_{c,i}) - \frac{\dot{V}(\sum[X_i]\hat{h}_{c,i})}{V} + \frac{p\sum[\dot{X}_i]}{\sum[X_i]} + \frac{\dot{m}_{ic}h_i + \dot{m}_{ec}h_e - \dot{m}_{ce}h_c}{V}}{(\sum[X_i]\hat{c}_{p,i}(T)) - p/T} \quad (20)$$

2.5 Combustion Chemistry Modeling using the Integrated Arrhenius Rate Threshold

The stoichiometric (equivalence ratio = 1) reaction of propane and air is considered, although other equivalence ratios can also easily be considered. The major products assumption is made, such that the global reaction for combustion can be written as:

$$C_3H_8 + 5O_2 + 18.8N_2 \rightarrow 3CO_2 + 4H_2O + 18.8N_2 \quad (21)$$

In order to capture the homogeneous auto-ignition process, a simple and intuitive approach, the Integrated Arrhenius threshold, is used to model combustion initiation. This methodology was introduced in (Shaver *et al.*, 2003) and compared to other approaches. The simplicity, accuracy and intuitive nature of the approach make it a very attractive low-order combustion chemistry model. In this approach, the rate of reaction of the propane is modeled as a Wiebe function following the crossing of an integrated Arrhenius rate, taking the form:

$$w_{rxn,C_3H_8} = \left\{ \begin{array}{ll} \frac{[C_3H_8]_i V_i \theta a(m+1)\left(\frac{\theta-\theta_i}{\Delta\theta}\right)^m exp\left[-a\left(\frac{\theta-\theta_i}{\Delta\theta}\right)^{m+1}\right]}{V\Delta\theta} & : \int RR \geq \int RR_{th} \\ 0 & : \int RR < \int RR_{th} \end{array} \right\} \quad (22)$$

where θ_i, V_i and $[C_3H_8]_i$ are the crank angle, volume and propane concentration, respectively, at the point where combustion begins (i.e. where $\int RR = \int RR_{th}$). The duration of combustion is $\Delta\theta$. The parameters a and m shape the Wiebe function.

The value of the integrated Arrhenius rate, itself, has the form:

$$\int RR = \int_{IVO}^{\theta} AT^n exp(E_a/(RT))[C_3H_8]^a[O_2]^b d\theta \quad (23)$$

where the threshold value of the integrated reaction rate, $\int RR_{th}$, has a value which correlates experiment and model at one operating condition. The values A, E_a/R, a, b and n are empirical parameters determined from propane combustion kinetics experiments. The values used here are $8.6e11(gmol/cm^3)^{(1-m-n)}/s$, $15,098K$, 0.1, 1.65 and 0, respectively (Turns, 2000). By inspection of Equation 21, the reaction rates of the other species are:

$$w_{rxn,O_2} = 5w_{C_3H_8} \quad (24)$$

$$w_{rxn,N_2} = 0 \quad (25)$$

$$w_{rxn,CO_2} = -3w_{C_3H_8} \quad (26)$$

$$w_{rxn,H_2O} = -4w_{C_3H_8} \quad (27)$$

The integrated Arrhenius rate threshold model directly relates the combustion phasing to the crank angle, θ_i, where the threshold value is first achieved. Then, the dependence of combustion phasing on the in-cylinder temperature, reactant concentrations and the point at which reactant charge is introduced in the cylinder (i.e IVO) is captured with Equation 23. Note that this approach differs from knock integrals used to model HCCI (Agrell *et al.*, 2003; Ohyama, 2000). The knock integral does not directly account for the reactant concentrations as is done in the technique used here. In the case where the amount of reactant inducted is the same from cycle-to-cycle, an approach like the knock integral would be appropriate. However, when this is not the case (i.e. when the reactant gas is being diluted by re-inducted or trapped product gas, during transients, or when operating over a range of conditions), an approach that accounts for reactant concentrations is more desirable.

The fact that reactant concentrations, temperature and valve timing influence the combustion phasing has already been identified in previous experimental work (Caton *et al.*, 2003). What the integrated Arrhenius rate approach does is provide a fairly simple model to describe this relationship between combustion phasing and parameters which are affected by the VVA system, namely: the inducted reactant concentrations, $[C_3H_8]$ and $[O_2]$; when they are initially introduced, IVO; and the temperature, T, of the mixture of reactants and re-inducted products.

2.6 Exhaust manifold modeling

The exhaust manifold model attempts to capture the thermodynamic properties of the reinducted exhaust gas by following the evolution of a variable amount of mass in the manifold. The relevant mass at any time includes the exhaust from the most recent cycle and a small residual, $m_{residual}$, from the previous exhaust cycle. Retaining this amount of mass from the previous cycle allows the internal energy to exist continuously and provides a means of modeling mixing between cycles.

Figure 2 shows the progression of mass in the exhaust manifold model. When the exhaust valve opens, flow through the valve increases the mass in the manifold until the piston reaches top dead center and reinduction begins. Reinduction similarly decreases the mass in the manifold until the point where the exhaust valve closes. After this point, the boundary defining the control volume smoothly resets to the residual mass, reflecting the fact that combustion products tend to flow away from the valve and exert less influence on the next reinduction. Mathematically, this model can be described by:

$$\dot{m}_e = \left\{ \begin{array}{rcl} \dot{m}_{ce} & : & EVO < \theta < 720 \\ -\dot{m}_{ec} & : & 0 < \theta < EVC \\ -\frac{m_{e,EVC} - m_{residual}}{EVO - EVC}\omega & : & EVC < \theta < EVO \end{array} \right. \quad (28)$$

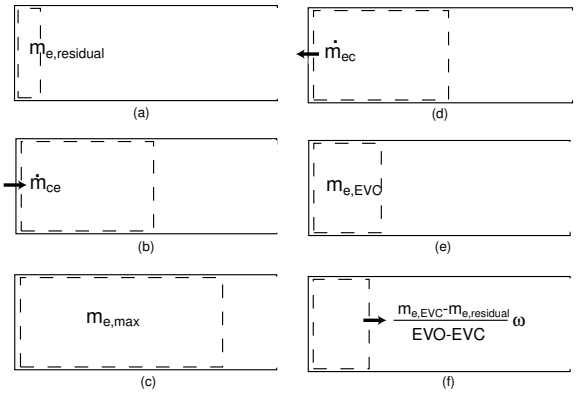

Fig. 2. Schematic of exhaust manifold control mass: (a) residual mass from previous exhaust cycle, $\theta = EVO$; (b) increase in mass due to cylinder exhaust, $EVO < \theta < 720$; (c) maximum amount of exhaust manifold mass, $\theta = 720$; (d) decrease in mass due to reinduction, $0 < \theta < EVC$; (e) post-reinduction mass, $\theta = EVC$; (f) decrease in mass to residual value, $EVC < \theta < EVO$

In order to obtain a governing expression for the exhaust manifold internal energy, u_e, the first law of thermodynamics is applied in conjunction with the ideal gas assumption and a simple convective heat transfer model. The first law of thermodynamics for product gases in the exhaust manifold is:

$$\frac{d(m_e u_e)}{dt} = \dot{Q}_e - \dot{W}_e + \dot{m}_{ce} h_c - \dot{m}_{ec} h_e \qquad (29)$$

where u_e is the internal energy of product gases in the manifold, $\dot{Q}_e = -\bar{h}_e A_e (T_e - T_{ambient})$ is the manifold heat transfer rate, where $\bar{h}_e$ is the convection coefficient of exhaust over the area, A_e, and $\dot{W}_e = p_{atm}\dot{V}_e$ is the boundary work for the control mass as it moves against atmospheric pressure.

The exhaust volume is related to the mass through the ideal gas assumption:

$$V_e = \frac{m_e R T_e}{MW_e p_{atm}} \qquad (30)$$

where MW_e is the molecular weight of the major products of combustion.

The temperature of the exhaust is a function of the internal energy, given that pressure is assumed to be constant at one-atmosphere.

$$T_e = f(u_e | p_{atm}) \qquad (31)$$

The enthalpy of the exhaust can be expressed as a function of the internal energy and temperature:

$$h_e = u_e + RT_e \qquad (32)$$

Combining 29, 30, 31 and 32 a governing equation for the internal energy of the gases in the exhaust manifold can be expressed as:

$$\dot{u}_e = \frac{1}{m_e \gamma}\left[\dot{m}_{ce}(h_c - h_e) + \bar{h}A(T_{ambient} - T_e)\right] \qquad (33)$$

Equations 1, 4, 20, 28 and 33 represent the set of nonlinear differential equations for each of the nine model states.

3. MODEL RESULTS WITH COMPARISON TO EXPERIMENT

3.1 Steady state operation

Figure 3 shows a comparison of simulated and experimental steady-state pressure-crank angle diagrams at two operating conditions. Note that the simulation results correlate quite well with the experiment. For details on the research engine, see (Caton *et al.*, 2003). For details on the VVA system, see (Hathout *et al.*, 2004). Averaged experimental pressure-crank angle diagrams are used because IC engine combustion processes inherently have some cycle-to-cycle dispersion. At this point, no process noise is added into the model to simulate the cyclic dispersion; however, nothing in the modeling strategy precludes the introduction of such a noise model.

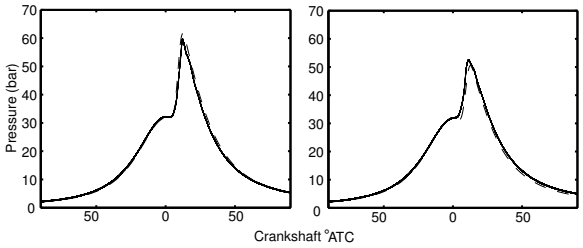

Fig. 3. Simulated HCCI combustion during steady state: dashed - simulation, solid - experiment; left - IVO/EVC=25/165, right - IVO/EVC=45/185

3.2 Transient operation

As noted previously, exhaust gas coupling exists between subsequent engine cycles when HCCI is achieved by re-inducting hot exhaust products with the VVA system. The modeling strategy outlined in this paper captures these dynamics with the inclusion of the exhaust manifold model presented in Section 2.6. Figure 4 shows simulation and experimental results of the in-cylinder pressure during a step change in the valve timing. Cycle 1 corresponds to the steady state solution at a valve timing of IVO/EVC$= 50/180$. A step change to a valve timing of IVO/EVC$= 70/185$ is then made. The simulation, though not exact, shows definite agreement with the general trend from experiment. The rippling on the expansion side of the experimental pressure curves is due to the fact that the auto-ignition process is not completely homogeneous, leading to modest pressure waves at higher loads.

Note the nonlinearity of the cyclic coupling, as combustion phasing occurs first earlier and then later as the system converges toward a steady state solution for the new valve timing. For this reason, it can be seen that appropriate valve timings depend not only on desired values of combustion phasing and load, but also on the previous cycle's behavior. Care must be taken to avoid misfire and erratic dynamics. In order to address these issues, a multi-cycle, model-based control strategy for HCCI Engines utilizing VVA is presented in (Shaver and Gerdes, 2003). The control strategy outlined there is validated using both the model presented in this paper and experiment.

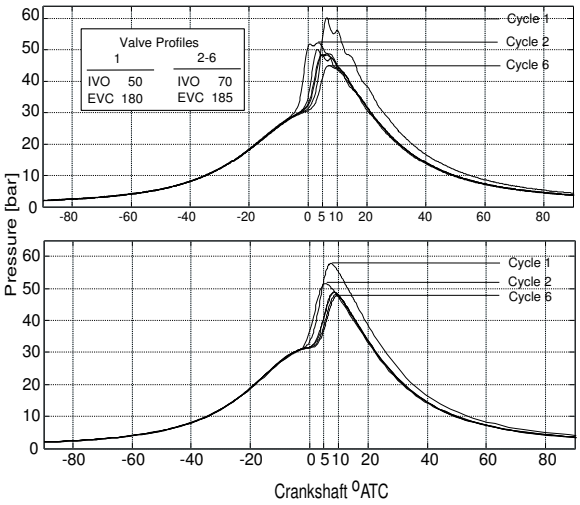

Fig. 4. Simulated HCCI combustion over a valve timing change: top - experiment, bottom - simulation

4. CONCLUSION

Homogeneous charge compression ignition engines have shown great promise to reduce NO_x emissions, while increasing efficiency. However, a critical control problem exists since the initiation of combustion is not directly controlled. Additionally, there exists cycle-to-cycle coupling through the exhaust gas for residual-affected HCCI engines outfitted with VVA. The work outlined in this paper extends modeling work completed previously by adding an exhaust manifold model to capture the cycle-to-cycle dynamics. This combination of a single zone combustion model, an integrated Arrhenius rate for ignition and a control mass exhaust manifold model accurately predicts the steady state and transient behavior.

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