CHEMICAL COMPOSITION MODELING OF A TWO-ZONE CONTROL-ORIENTED MIXING MODEL FOR HOMOGENEOUS CHARGE COMPRESSION IGNITION ENGINES

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ABSTRACT
Due to the need for clean and efficient automobile propulsion systems, this paper models an important process in the enabling of homogeneous charge compression ignition (HCCI) engines. The need for a deep understanding of charge-residual mixing in residual-affected HCCI engines requires a model of the chemical composition during the mixing process. In this paper, a chemical composition model is developed specifically for a two-zone mixing model to account for important phenomena such as the presence of unburned fuel in the residual exhaust gas. The model is developed as a control-oriented model that can be used for real-time decision making and control. This paper develops the composition model for the major species present, and also presents the method that would be used to include other minor species. The model is simulated for variations in residual gas fraction equivalence ratio, a misfire situation, and its effects on air/fuel ratio.

INTRODUCTION
The need for better stewardship of our energy resources has become clear with concerns over environmental impact and more stringent governmental regulation. In the sector of personal transportation, where the four-stroke internal combustion engine is dominant, there are two approaches to reducing environmental impact. The first is to replace the internal combustion engine, such as with electric vehicles and hydrogen fuel cells. The second approach is to improve the efficiency of the internal combustion engine. One technology that fits into this second category is Homogeneous Charge Compression Ignition (HCCI) [1].

HCCI is an advanced engine technology that promises a 15-20% improvement in the efficiency over a standard, gasoline-fueled, spark ignition (SI) engine, with significant improvements in particulate and NOx emissions. [1][2] HCCI operates by compressing a fuel and air mixture until it reaches its autoignition point. The mixture combusts quickly and at low temperature without a flame front. Since there is no flame front (as in SI engines), combustion temperatures are lower, thus reducing NOx emissions. The homogeneous nature of the mixture lowers the particulate emissions.

The major challenge of HCCI is controlling combustion. Unlike SI and compression ignition engines (which have direct initiators of combustion), HCCI has no distinct event that controls combustion timing. Combustion timing is determined by the thermodynamic state at intake valve closing (IVC). Therefore, to control combustion, temperature, pressure, and composition must be controlled to set the conditions at IVC.

A method of controlling conditions at IVC is to use hot, residual exhaust gas, and blend the exhaust with the fresh charge. The ratio of the hot residual to the cool, fresh charge determines the overall mean temperature at IVC [3]. This model considers negative valve overlap (NVO, also known as recompression), where exhaust gas is trapped during the exhaust stroke of the engine by closing the exhaust valves before the piston reaches top dead center (TDC), thus preventing all of the exhaust from being expelled from the cylinder.

Currently, two main approaches to modeling and controlling HCCI exist within the field. The first uses single-zone models for combustion modeling. In [4], the authors develop a mean-value model for HCCI combustion using an Arrhenius integral method. In [5], the authors develop a single-zone HCCI model suitable for control systems. A significant advantage of single-zone models is their relative simplicity,
thus making them well suited for real-time control applications. However, single-zone models cannot capture the in-cylinder fluid and chemical dynamics precisely.

The second approach to HCCI modeling uses numerical methods and Computation Fluid Dynamics (CFD). By dividing the cylinder into a large number of zones, the model is able to capture the fluid and chemical dynamics occurring within the cylinder during each stroke [6][8]. In [6], the authors present an investigation of the effects of valve timings on in-cylinder fluid behavior. A major disadvantage to the CFD methods is their complexity and time-consuming nature. These characteristics make them unsuitable for real-time control.

Real-time control is a critical component of HCCI. Realizing HCCI using exhaust gas requires precise control of the cylinder inputs—fuel and air—using systems such as fully flexible valve actuation systems [7], [9]. However, the degree of mixing between residual exhaust gas and fresh charge has a significant effect on combustion [10]. In [10], the authors have presented a novel valve strategy where the intake valves are operated asynchronously. Through their work in [10], and previous work in [11], they have demonstrated the effect that mixing can have on combustion.

In [12], we have developed a two-zone mixing model for HCCI combustion. The advantage of this model is that it is able to capture complex mixing dynamics in a tractable model suitable for real-time control. In this paper, we utilize this model to develop a chemical composition model that describes the behavior of the chemical composition in an HCCI engine subject to the novel NVO strategy presented in [10].

TWO-ZONE MIXING MODEL

The goal of the two-zone mixing model in [12] is to capture complex flow characteristics in a complete and tractable model, while keeping computational time in line with that of the phenomenological models. Some details of this model are presented here in order to show the connection to the chemical composition model developed here.

Modeling the flow processes with one or two zones can be risky. Certain fluid mixing behaviors are best described by CFD techniques. By reducing the dimensions of the model, we risk ignoring important behaviors. However, knowledge of overall flow behavior and its effects on combustion can inform our development of a control-oriented model. A model presented in [13] utilizes two distinct regions for the combustion model, and determines the chemical composition of each region. The model in [13] only considers composition as it relates to the average temperature, by assuming a known zonal mass distribution and complete combustion. The work in this paper specifically looks unburned fuel in the composition of the mixture. In [14] the authors present a detailed chemical composition model for HCCI combustion, however, it is for single-zone model and thus cannot include mixing effects.

\[\dot{m}_1 = \dot{m}_1 + \dot{m}_{\text{rtm}} \]  
\[\dot{m}_2 = -\dot{m}_{\text{rtm}}. \]

The size of Region 1 is the quantity of interest, as it will be used as an input for a combustion model.

The rate of growth of Region 1, \(\dot{m}_{\text{rtm}}\), is a function of the flow characteristics at the intake valves. Properties that alter \(\dot{m}_{\text{rtm}}\), and therefore the mixing within the cylinder, are velocity of the inlet flow and the quantity of residual mass present in the cylinder:

\[\dot{m}_{\text{rtm}} = \frac{\rho v^2_{\text{IVO}} A_{\text{m}} (V_2 - V_{\text{IVO}})}{A_{\text{m}} T_{\text{rgf}} C_p} \]

In Eq. (2), \(\rho\) is the fluid density, \(v_{\text{IVO}}\) is the inlet flow velocity, \(A_{\text{m}}\) is the open valve area, \(A_{\text{rgf}}\) is the cylinder area, \(T_{\text{rgf}}\) is the residual temperature, \(V_2\) is the volume of Region 2, \(V_{\text{IVO}}\) is the...
volume of the cylinder at IVO, and \( c_p \) is the specific heat. Derivation of Eq. (2) can be found in [12].

**DETERMINATION OF CHEMICAL COMPOSITION OF THE TWO-ZONE MIXING MODEL**

An important component of the two-zone model is the determination of the chemical composition within the cylinder and the effects of composition on the combustion process. While the typical assumption for single-zone models of HCCI combustion is that there is not an appreciable amount of unburned fuel at the end of the combustion process, using a residual affected control strategy necessitates an examination of the composition of the exhaust gas. This is because with an NVO strategy, exhaust components from one cycle are recycled into the next engine cycle. Thus, if there are any products (such as unburned fuel) in the exhaust, they will have some effect on the subsequent combustion.

Even though many single-zone models of HCCI ignore unburned fuel in the residual, there is some precedent in assuming that the combustion reaction does not go to completion. In [4], the author’s define the end of combustion as the timing when 90% of the fuel has burned. The remaining amount of fuel (10% in this case) is a major motivation in developing the chemical composition characteristics of the two-zone model.

**Chemical Composition Model Set-up**

For this model, octane (C\(_8\)H\(_{18}\)) is used as the fuel, and air is assumed to be (O\(_2\)+3.76N\(_2\)). The species considered for the reaction include the major species of: octane, diatomic oxygen (O\(_2\)), diatomic nitrogen (N\(_2\)), water vapor (H\(_2\)O), carbon dioxide (CO\(_2\)), and carbon monoxide (CO). These are not the only species present during the reaction, however, but in the interest of reducing computational burden, the number of species can be limited to these six without a significant loss of accuracy [16]. This is not to say, however, that other species cannot be included in this model. It will be shown, that with the inclusion of carbon monoxide, species beyond these major species can account for.

Accounting for the presence of residual, a global reaction can be expressed as Eq. (3):

\[
aC_8H_{18} + bO_2 + cN_2 + dH_2O + eCO_2 + fCO \rightarrow \\
\alpha C_8H_{18} + \beta O_2 + \nu N_2 + \psi H_2O + \sigma CO_2 + \mu CO
\]

where the coefficients of the species are the stoichiometric coefficients as the reaction proceeds from reactants to products. For Region 1, there is a mixture of fresh charge and residual. We define \( x_r \), the residual gas fraction, as follows:

\[
x_r = \frac{m_r}{m_r + m_g}
\]

where \( m_r \) is the mass of the retained residual gas and \( m_g \) is the mass of the fresh charge. The equivalence ratio, \( \phi \), is defined as:

\[
\phi = \frac{\lambda}{\lambda_r}
\]

Where \( \lambda \) and \( \lambda_r \) are defined as the air/fuel ratio and the stoichiometric air/fuel ratio, respectively. Thus, the coefficients of the reactants can be written in terms of \( x_r \) and \( \phi \):

\[
a = 1 + \alpha x_r
\]

\[
b = \frac{12.5}{\phi} + \beta x_r
\]

\[
c = \frac{47}{\phi} + \nu x_r
\]

\[
d = \psi x_r
\]

\[
e = \alpha x_r
\]

\[
f = \mu x_r
\]

An assumption is that that the coefficient \( a \), which is the fraction of fuel that is not burned during combustion, can be reasonably estimated. For instance, one would set \( a \) as 0.1 if it were assumed that combustion ends with 90% of fuel burned. In Eqs. (6) – (8), the first term represents the fresh charge and the second term represents the amount of recycled residual. Equations (9) – (11) are only functions of the recycled residual.

The remaining coefficients can be related using a species-mass balance. This process solves for the coefficients by setting up equalities for each element in the chemical reactions (carbon, hydrogen, oxygen, and nitrogen). Since elements must be conserved, one equation is created for each element present. However, this only gives 4 equations with 5 unknowns \( (\beta, \nu, \psi, \sigma, \mu) \). Typically, in lean mixtures, carbon monoxide can be ignored as a product [16]. Doing so, it leads to the following equation for the chemical reaction:

\[
\left(1 + \alpha x_r\right)C_8H_{18} + \left(\frac{12.5}{\phi} + \beta x_r\right)O_2 + \left(\frac{47}{\phi} + \nu x_r\right)N_2
\]

\[
+ \psi x_r H_2O + \alpha x_r CO_2 + \mu x_r CO \rightarrow
\]

\[
\alpha C_8H_{18} + \beta O_2 + \nu N_2 + \psi H_2O + \sigma CO_2 + \mu CO
\]

\[
\beta = \frac{12.5}{\phi(1-x_r)} + \frac{(x_r-1)[25(1+\alpha x_r)-34\alpha]}{2(1-x_r)^2}
\]
\[
\nu = \frac{47}{\phi(1-x_r)} \tag{14}
\]
\[
\psi = \frac{9(1+\alpha x_r)-18\alpha}{1-x_r} \tag{15}
\]
\[
\sigma = \frac{8(1+\alpha x_r)-8\alpha}{1-x_r} \tag{16}
\]
\[
\mu = \theta (\text{Ignoring CO}) \tag{17}
\]

From Eqs. (12) – (17), we now have a description of the chemical composition of Region 1 in terms of known quantities: the residual gas fraction, equivalence ratio, and the estimate of the combustion completeness. From this we are able to monitor the progression of the composition of the mixture. A similar procedure can be implemented to compute the composition in Region 2.

**Chemical Composition with Cycle-to-cycle Dynamics**

The global chemical composition Eq. (12) can be further developed to indicate the cycle-to-cycle dynamics of composition with regard to the two-zone mixing model. We consider cycle \(i\) with respect to the previous cycle, \(i-1\). The residual gas fraction, \(x_r(i)\), for the \(i\)-th cycle is defined as using the residual gas from the \(i-1\) cycle, but being applied to the current \(i\)-th cycle. The global Eq. (3) is rewritten as:

\[
a(i)C_nH_{18} + b(i)O_2 + c(i)N_2
+ d(i)H_2O + e(i)CO_2 \rightarrow
\]
\[
\alpha(i)a(i)C_nH_{18} + \beta(i)O_2 + \nu(i)N_2
+ \psi(i)H_2O + \sigma(i)CO_2 \tag{20}
\]

The reactant coefficients must be defined in terms of the output of cycle \(i-1\).

\[
a(i) = 1 + \alpha(i-1)a(i-1)x_r(i) \tag{21}
\]
\[
b(i) = \frac{12.5}{\phi(i)} + \beta(i-1)x_r(i) \tag{22}
\]
\[
c(i) = \frac{47}{\phi(i)} + \nu(i-1)x_r(i) \tag{23}
\]
\[
d(i) = \psi(i-1)x_r(i) \tag{24}
\]
\[
e(i) = \sigma(i-1)x_r(i) \tag{25}
\]

As with Eqs. (13) – (17), the coefficients of the products can be determined by a species-mass balance.

\[
a(i) = 1 + \alpha(i-1)a(i-1)x_r(i) \tag{26}
\]
\[
\beta(i) = \frac{12.5}{\phi(i)} + x_r(i)\beta(i-1)
-12.5[1-\alpha(i)]\left[1+\alpha(i-1)a(i-1)x_r(i)\right] \tag{27}
\]
\[
\nu(i) = \frac{47}{\phi(i)} + \nu(i-1)x_r(i) \tag{28}
\]
\[
\psi(i) = 9[1-\alpha(i)]\left[1+\alpha(i-1)a(i-1)x_r(i)\right] + \psi(i-1)x_r(i) \tag{29}
\]
\[
\sigma(i) = 8[1-\alpha(i)]\left[1+\alpha(i-1)a(i-1)x_r(i)\right] + \sigma(i-1)x_r(i) \tag{30}
\]

To account for the two-zone mixing model, the mole fraction of each species must be computed. For the coefficients of each reactant species, \(q \in \{a,b,c,d,e\}\), the mole fraction of each species in Region \(n\) is \((n \in \{1,2\})\):

\[
\chi_n^q = \frac{N_n^q}{N_n^t} \tag{31}
\]

where \(N_n^q\) is the coefficient \(q\) in Region \(n\), and \(N_n^t\) is the sum of the coefficients in Region \(n\). Similarly, for coefficients in the product phase, \(s \in \{\alpha,\nu,\beta,\psi,\sigma\}\), the mole fraction is

\[
\chi_p^s = \frac{N_p^s}{N_p^t} \tag{32}
\]

The mass fraction of a species \(u\) in Region \(n\), is defined as

\[
y = \chi_n^u \frac{M_u}{M^t}\] where \(M^t\) is the molecular weight of species \(u\) and \(M^t\) is the total molecular weight of the mixture. To find the amount of a species in the \(i\)-th cycle, the contribution of both the intake charge and the residual gas must be considered. After the intake process, \(m_{rm}\) is the amount of residual from Region 2 that has transferred to Region 1. If the fresh charge is in state \(fc\) prior to mixing, then the mass of the fuel in Region 1 in cycle \(i\) is determined as follows:

\[
m_i^t(i) = m_i(fc)\gamma_i^t(i) + m_{rm}(i)\gamma_i^{rm}(i) \tag{33}\]

In Eq. (33), the first term is the mass of fuel in the fresh charge, and the second term is the amount of fuel in the residual transferred from Region 2 to Region 1. Similar relationships for other species in Region 1 are as follows:
\[ m^b(i) = m_b(i) + m_{\text{rem}}(i)y^b_r(i) \] (34)

\[ m^c(i) = m_c(i) + m_{\text{rem}}(i)y^c_r(i) \] (35)

\[ m^d(i) = m_{\text{rem}}(i)y^d_r(i) \] (36)

\[ m^e(i) = m_{\text{rem}}(i)y^e_r(i) \] (37)

With Eqs. (20) – (37), we have the composition of each species as a function of the products from the previous cycle. This is critical for the development of HCCI and its enabling technologies (camless valve actuation, high-pressure direct injection, etc.) because this model allows for intervention on the cycle-to-cycle timeframe, and thus increasing the potential for greater stability in HCCI.

**Composition with Minor Species**

In the previous sections, we ignored carbon monoxide as a product. One reason for this is that for a lean mixture, carbon monoxide can usually be ignored [16]. However, we will use carbon monoxide to illustrate the procedure for including more species than those used in the previous section. With CO now in the chemical Eq. (3), one more relationship is required in order solve for the coefficients. For this, we look at the equilibrium of oxygen, carbon monoxide, and carbon dioxide:

\[ \text{CO}_2 \leftrightarrow \text{CO} + \frac{1}{2}\text{O}_2 \] (38)

The equilibrium constant \( K_p \) for the reaction in Eq. (38), can be expressed as:

\[ K_p = \frac{\rho \beta^2}{\sigma} \left( \frac{P(\theta)}{\beta + \sigma + \mu} \right)^{\frac{1}{2}} \] (39)

where \( P \) is the cylinder pressure at any crank angle \( \theta \). The equilibrium constant \( K_p \) can be determined by one of two methods. The first is to use tabulated values. This method is preferred because of the simplicity, but tabulated values are readily available only for common equilibrium equations such as Eq. (38). The method for calculating the equilibrium composition aside from tabulated values will be detailed so that it may also be applied to minor species and radicals whose equilibrium constants are not readily available can be considered. Therefore, defining the equilibrium constant as:

\[ K_p = e^{-\frac{\Delta G^*(T)}{RT}} \] (40)

In Eq. (40), \( \Delta G^*(T) \) is the Gibbs function as a function of temperature, \( T \), and \( R \) is the universal gas constant. The Gibbs function can be calculated using standard properties of compounds, as detailed in [17]. Once an expression for the Gibbs function is obtained, the equilibrium constant can be expressed as a function of temperature. However, calculating the Gibb’s function is an iterative and time consuming process. Further complicating matters is that the temperature (and thus the equilibrium composition) changes continuously through the engine cycle, and so the Gibbs function must be iterated at each temperature value. Also, the resulting equations for the stoichiometric coefficients will be a second order function of temperature and species concentration. It would thus be possible to solve for the coefficients, but because of the need to iterate the Gibb’s function at each temperature, and solve the second order function, the process becomes computationally intensive. As more species are added, the computational burden increases, making real-time control harder to achieve.

**RESULTS OF CHEMICAL COMPOSITION SIMULATION**

The above chemical composition model was simulated under conditions where the equivalence ratio and residual gas fraction were changed. The information from these simulations would become part of a combustion simulation using an Arrhenius integral method [12], [4].

![Figure 2. Simulation of chemical composition with a variation in equivalence ratio (dashed red line on lower plot).](image-url)
For a change in residual gas fraction, the amount of species will change correspondingly (Figure 3). In this simulation, the residual fraction is varied among 10%, 30%, and 5%, with the equivalence ratio held constant at 0.9. When the residual gas fraction changes, there is a delay of approximately 4 cycles until the composition has stabilized at the new value.

A misfire was also simulated (Figure 4). To accomplish this, at a particular time (cycle 40), the amount of unburned fuel was increased to 100% while the equivalence ratio was held constant at 0.9. In this case, the combustion products (water and carbon dioxide) reduce to 0 moles and the amount of product oxygen increases to the amount that is inducted (because none of it is consumed). The misfire is then recovered by altering the residual gas fraction to increase the temperature. The amount of unburned fuel reduces to zero, and combustion destabilizes. The control strategy utilized is a hand-tuned method; however, the behavior of composition is as predicted.

To determine the effect of the chemical composition model on the two-zone HCCI combustion model, the combustion model was simulated with the chemical composition model turned off, then turned on. The case where the valves were operated asynchronously (i.e., the second intake valve is opened 15 CAD later) is shown in Figure 5. The air/fuel ratio is plotted against injected fueling amount, and the simulation was run for a number of IVO timings (between 20 CAD aTDC and 50 CAD aTDC). The variation in IVO timings causes the residual fraction to vary between 4% and 15%. When using the chemical composition model, the AFR decreases by approximately 12% at 3 mg of fuel (low load) and 11% at 6 mg of fuel (high load). This indicates that the composition model is predicting the transfer of fuel and oxygen from Region 2 to Region 1, and that this fuel is affecting the subsequent combustion. Compared to synchronous valve operation, the AFR is 1-2% less for the asynchronous case, indicating that the improved mixing, and thus greater amount of transfer from Region 2 to Region 1, is affecting the AFR as predicted by the combustion model.

CONCLUSIONS

The chemical composition behavior in the two-zone mixing model for charge-residual mixing provides a critical component in the enabling of HCCI. As we gain more and more control over the engine cycle through enabling technologies, the need for accurate models describing complex processes is very clear. With the ability to model composition, we can account for various factors with temperature and unburned fuel in the two-zone dynamic model. Simulation results show that this model behaves as expected for various changes in equivalence ratio and residual gas fraction, as well nontraditional events such as misfire. The model is also able to predict the change in fuel and air when compared to a two-zone model without consideration of chemical composition.
The next steps in the development of this model will be a validation method that includes both numerical simulation and experimental verification. Computational fluid dynamics (CFD) software will be used to verify the mixing model, and when combined with chemical kinetic simulation, it is a means of validation for this chemical model. Experimental validation will be performed by integrating various enabling technologies (camless valve actuation, high-pressure direct injection, and a sophisticated control system) to run an ICE with a focus on the mixing process. For these purposes, an optical engine will be used. Also, the stability, controllability, and observability of this model will be determined analytically. Since the model is highly non-linear, analytical solutions for these three characteristics is non-trivial, a thus careful examination must be afforded to an analytical solution.

REFERENCES


