

Sensitivity Analysis of Combustion Timing of Homogeneous Charge Compression Ignition Gasoline Engines

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The goal of this paper is to identify the dominant factors that should be included in a control oriented model in order to predict the start of combustion in a homogeneous charge compression ignition (HCCI) engine. Qualitative and quantitative information on the individual effects of fuel and exhaust gas recirculation on the HCCI combustion is provided. Using sensitivity analysis around a wide range of operating conditions of a single-cylinder port-injection gasoline HCCI engine, we find that temperature is the dominant factor in determining the start of combustion. Charge temperature thus becomes the “spark” in a HCCI engine. Therefore, a model without the composition terms should be adequate for model based regulation of the combustion timing in a port-injection gasoline HCCI engine with high dilution from the exhaust. [DOI: 10.1115/1.2936877]

1 Introduction

The basic idea of homogeneous charge compression ignition (HCCI) engines is the autoignition of a homogeneous mixture that is sufficiently lean to keep peak combustion temperatures below 1700 K such that low NO_x and low particulate matter (PM) emissions are achieved [1]. Due to the high compression ratio (CR) required to initiate the combustion and the rapid heat release process, HCCI engines also achieve high thermal efficiency [2]. As a result, HCCI engines achieve fuel economy levels comparable to that of compression ignition (CI) engines, while generating engine-out NO_x emissions that are as good as tailpipe NO_x emissions from conventional spark ignition (SI) engines with after treatment [1]. Therefore, the HCCI engine is a promising option for a clean and efficient configuration of internal combustion engine.

One of the key difficulties in the implementation of HCCI technology in production engines is that ignition cannot be directly actuated. The timing of autoignition of HCCI combustion is determined by the cylinder charge conditions, rather than the spark timing or the fuel injection timing that are used to initiate combustion in the SI and CI engines, respectively [3]. As demonstrated by many experimental results [4,5], controlled autoignition requires regulation of the charge properties, namely, temperature, pressure, and composition at the intake valve closing (IVC). Once

the valves are closed, there is very little that can be done to affect ignition. Hence, all the controllable engine variables need to be adjusted prior to IVC in a judicious way based on accurate predictions of their influence on combustion timing. To regulate the HCCI combustion phasing, as in Refs. [6] and [7], an accurate model for the start of combustion timing (SOC) is necessary. Analysis in Ref. [8] has shown that the autoignition modeling approach has significant potential for gasoline engine application but will require calibration for accuracy over the full range of engine operation. These models will be used for feedforward and feedback control design, which sometimes rely on inversion of the modeled input-output relationships. It is thus important to avoid overdetermined models, which can indicate multiple possible combination of engine variables for the same combustion characteristics. Minimal parametrizations avoid the extra complexity of having to eliminate nonrealizable combinations of engine variables and enable easy calibration of the controllers in a production-intent application.

In this paper, we use sensitivity analysis to identify which factors have a dominant effect on and should be included in the SOC model. Existing single-zone models for autoignition timing of iso-octane are examined for their ability to predict gasoline ignition. The sensitivity analysis is conducted around a wide range of operating conditions in a single-cylinder gasoline engine with varying fuel and exhaust gas recirculation (EGR). Similar analysis for the combustion duration can be found in Refs. [9] and [10]. Our conclusions corroborate results of a simulation study based on an engine model with detailed chemical kinetics calibrated with a four-stroke single-cylinder engine fueled with iso-octane [11]. In addition, the thermal dominance in controlling ignition timing using high internal dilution revealed by our study is consistent with the conclusion reached by Najt et al. in Ref. [5] by experimentally exploring the effects of several parameters on the ignition process of a HCCI engine.

Section 2 introduces the experimental configuration and shows that the test conditions considered in this paper cover a wide range of load, exhaust dilution, equivalence ratio, and temperature under constant engine speed. In Sec. 3, the mechanism of combustion initiation is explained by the generation of radicals from a chain reaction. We summarize two models for SOC [12,13], both of which are able to predict ignition in a gasoline engine. The model in Ref. [13] contains the concentration effect for iso-octane and is parametrized using the pressure time history generated by a rapid-compression facility (RCF). The model in Ref. [13] has been used in Ref. [14] to predict ignition timing in a single-cylinder gasoline engine. The model in Ref. [12] depends only on temperature and is calibrated and validated with experimental data from a single-cylinder gasoline engine. In Sec. 4, we analyze the sensitivity of the model in Ref. [13] to determine which parameters are the most important for prediction of the autoignition timing. The effect of temperature and composition on the ignition timing through changes in the hot dilution in the cylinder is studied. We find that temperature has dominant impact in a wide range of operating conditions with different fuels and EGRs.

The fact that temperature (not composition) is the dominant mechanism for controlling the combustion, timing has a direct implication for system stability and controller design. Specifically, the residual gas trapped in the cylinder of a HCCI engine constitutes an internal thermal feedback loop, which affects the stability of the temperature dynamics as analyzed in Ref. [15]. An intelligent control design accounting for the temperature dynamics is necessary to stabilize the HCCI engine under certain conditions, such as during large load changes [16].

2 Experimental Conditions

Dynamometer experiments used in this study were performed on a single-cylinder and port-injection gasoline engine with a displacement of 550 cm^3 and CR of 13.75. The data were used in Ref. [12] to parametrize a HCCI combustion model, which was

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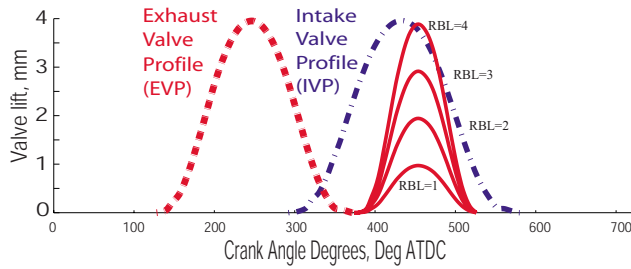
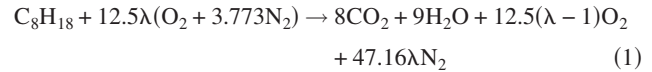


Fig. 1 Exhaust, intake and rebreathing valve profiles

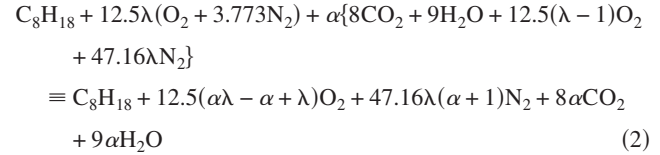
able to represent all the data available without using composition as a parameter. In this paper, we use the same data and parameterize models that include composition so that a sensitivity analysis can be performed. We summarize here a few of the key characteristics of the experimental data and conditions under which they were collected. More details can be found in Ref. [12].

The external intake air was heated to 90°C, which allowed HCCI engine operation at low fueling rates and buffered the engine from ambient temperature changes. This charge heating can be obtained by using a water-to-air heat exchanger in the intake similar to turbocharged engines. The dilution of the experimental gasoline engine was controlled by an actuation called rebreathing lift (RBL), which is a second opening of the exhaust valve during the intake stroke, as shown in Fig. 1. The steady-state data available can be categorized into two groups: Test A and Test B. In Test A, RBL is increased when fuel is decreased in order to achieve the largest operating load range at 1000 rpm. Specifically, data are collected at a constant speed of 1000 rpm and a range of load from 2.1 bars to 4.8 bars indicated mean effective pressure (IMEP), which corresponds to fueling levels from 7 mg/cycle to 15 mg/cycle. In Test B, RBL is varied while the amount of fuel is fixed at 11 mg/cycle in order to investigate the effect of internal exhaust dilution on combustion timing.

The charge composition is calculated based on the air-to-fuel ratio and the percentage of dilution achieved in the engine by physically changing actuated variables, such as the fuel and the RBL. In the rebreathing strategy, the cylinder charge temperature and composition are changed simultaneously by the hot recirculated exhaust gas. For instance, an increase in RBL brings more hot exhaust into the cylinder and thus results in a higher temperature at IVC and reduced fuel and oxygen concentrations. Iso-octane (C₈H₁₈) mixture is used in this paper to analyze the composition of each operating point observed at the gasoline HCCI engine since iso-octane is one of the primary reference fuels that determine octane numbers and knocking tendencies of gasoline mixtures under SI operating conditions. Moreover, the chemical kinetics of engine knock are very similar to the kinetics of ignition under HCCI conditions [17]. Experiments have shown that iso-octane behaves very much like gasoline except that iso-octane requires a slightly higher temperature to ignite [8,18]. Trendwise, iso-octane closely resembles gasoline. To calculate mole fractions of fuel and oxygen ($\chi_{C_8H_{18}}$ and χ_{O_2}) inside the cylinder, we consider first the global reaction of the combustion of iso-octane,



where λ is the relative air-to-fuel ratio, which is the ratio of actual to stoichiometric air-to-fuel ratio. It is a measure of the relative amounts of oxidizer (air) and fuel (C₈H₁₈) in the fresh charge inducted through the intake. The mixing of the fresh charge and reinducted product during the induction process for lean or stoichiometric iso-octane HCCI can then be represented as



where $\alpha \equiv N_{egr}/N_{frsh}$, which is the ratio of the moles of reinducted product N_{egr} to the moles of inducted fresh charge N_{frsh} [6]; it is a function of the RBL. Thus, the mole percent of the fuel C₈H₁₈ and oxygen O₂ can be computed

$$\chi_{C_8H_{18}} = \frac{N_{C_8H_{18}}}{N_{total}} = \frac{1}{59.66\alpha\lambda + 4.5\alpha + 59.66\lambda + 1} 100\% \quad (3)$$

$$\chi_{O_2} = \frac{N_{O_2}}{N_{total}} = \frac{12.5(\alpha\lambda - \alpha + \lambda)}{59.66\alpha\lambda + 4.5\alpha + 59.66\lambda + 1} 100\% \quad (4)$$

and the in-cylinder equivalence ratio can be expressed as

$$\Phi_c = (\chi_{C_8H_{18}}/\chi_{O_2})/(\chi_{C_8H_{18}}/\chi_{O_2})_s = (\alpha\lambda - \alpha + \lambda)^{-1} \quad (5)$$

where the subscript s represents the stoichiometric condition. With the information above, we can compute the respective $\chi_{C_8H_{18}}$, χ_{O_2} , and Φ_c using λ and α from the experimental data. The computed $\chi_{C_8H_{18}}$, χ_{O_2} , and T_{IVC} can then be substituted into the model in Sec. 3 for the model validation and sensitivity analysis. Table 1 summarizes the range of important variables in the two steady-state experiments. In both tests, engine speed and relative air-to-fuel ratio from the intake are held constant ($\lambda=1.4$). The air-to-fuel ratio and, hence, the equivalence ratio Φ_c in the cylinder, however, are changing due to the recirculated unburned oxygen. In Test A, a large HCCI load range (2.1 bars to 4.8 bars IMEP) at 1000 rpm is achieved by changing both fuel and RBL. The exhaust dilution, which is defined as the percentage of recirculated exhaust gas in the cylinder, varies from 35% to 67%. On the other hand, limited operating range is observed in Test B when RBL is changed while fuel is kept fixed.

3 Chain Reaction for Combustion Initiation

The combustion process is itself a chain reaction, the initiation of which is characterized by a substantial concentration of radicals from stable species [19]. Radicals are molecules with an unpaired electron such as O, OH, N, and CH₃. Therefore, a flammable mixture of fuel F and O₂ reacts and generates the radicals $R\cdot$: $F + O_2 \rightarrow R\cdot + \dots$, for example, $CH_4 + O_2 \rightarrow CH_3 + HO_2$. The production rate of the radicals $R\cdot$ is then represented in the Arrhenius form

Table 1 Summary of important variables in the steady-state experiments

Expt.	IMEP (bar)	Exhaust Dilution (%)	λ	Φ_c	$\chi_{C_8H_{18}}$ (%)	χ_{O_2} (%)	T_{IVC} (K)
Test A	2.1 to 4.8	35 to 67	1.4	0.47 to 0.62	0.4 to 0.8	10 to 15	440 to 480
Test B	3.5 to 3.6	45 to 50	1.4	0.55 to 0.57	0.55 to 0.65	12.6 to 13.7	458 to 470

$$\frac{d[R\cdot]}{dt} = \kappa[F]^a(t)[O_2]^b(t)p_c^n(t)\exp\left(-\frac{E_a}{RT_c(t)}\right) \quad (6)$$

where T_c and p_c are the cylinder temperature and pressure, respectively, κ is the preexponential factor, E_a is the activation energy for the reaction generating the radicals, and n , a , and b indicate the reaction's sensitivity to pressure and concentration of fuel and oxygen, respectively. At the IVC of a port-injection internal combustion engine, the radicals are negligible $[R\cdot](t_{IVC})=0$. Integration of Eq. (6) from t_{IVC} until the combustion is initiated t_{SOC} corresponds to a critical value of the concentration of radicals $[R\cdot]_c$,

$$[R\cdot]_c = \int_{t_{IVC}}^{t_{SOC}} \kappa[F]^a(t)[O_2]^b(t)p_c^n(t)\exp\left(-\frac{E_a}{RT_c(t)}\right)dt \quad (7)$$

Therefore, the combustion timing of an autoignition process can be described as an integral that sums up the reaction rate of radicals until the concentration of radicals reaches a critical value [17]. The initiation of combustion can be defined as the time when 1% of the fuel is burned t_{CA01} similar to the ignition delay in SI engines [20]. Since only 1% of the fuel is burned during the process, the chemical concentration (mole fraction) $[F]$ and $[O_2]$ can be considered constant throughout the interval t_{IVC} to t_{SOC} and equal to the concentrations at IVC. Furthermore, the factor κ is assumed to be independent of pressure and temperature since the largest contribution to the integral is made near the high pressure and high temperature when autoignition occurs [17]. Based on all of the assumptions above, the Arrhenius integral (8) used to predict the SOC should theoretically depend on the mixture composition (fuel and air) at IVC as indicated by many other researchers [13,21]:

$$AR = \int_{t_{IVC}}^{t_{SOC}} \kappa[F]^a(t_{IVC})[O_2]^b(t_{IVC})p_c^n(t)\exp\left(-\frac{E_a}{RT_c(t)}\right)dt \quad (8)$$

In Ref. [13], a specific correlation of composition, pressure, and temperature was identified for predicting the ignition delay time from the end of compression to the start of combustion using a RCF with iso-octane, oxygen, nitrogen, and argon mixtures. The functional form of the ignition delay identified in Ref. [13], was shown to represent experimental data from a single-cylinder gasoline engine at General Motors in Ref. [9] and concurrently but independently in Ref. [14] using another single-cylinder engine at the University of Michigan. The inverse of the ignition delay time identified in Ref. [13] becomes the integrand of the Arrhenius integral [17] with the subscript PTC indicating the correlation of pressure, temperature, and composition

$$\begin{aligned} AR_{PTC} &= \int_{\theta_{IVC}}^{\theta_{SOC}} \frac{1}{\tau_{PTC}N} \frac{60}{360} d\vartheta \\ &= \int_{\theta_{IVC}}^{\theta_{SOC}} 1264.5 \left(\frac{\chi_{O_2}}{\chi_{C_8H_{18}}} \right)_s^{0.77} \chi_{C_8H_{18}}^{0.77} \chi_{O_2}^{0.64} p_c^{1.05} \\ &\quad \times \exp\left(\frac{-141095}{R(1.09T_c)}\right) d\vartheta \end{aligned} \quad (9)$$

Note that assuming only small variations in engine speed during the period IVC \rightarrow SOC, we change the integration argument from the time domain (t) to the crank angle domain (ϑ). The parameter τ_{PTC} is the ignition delay time [s] identified in Ref. [13]; N is the engine speed (1000 rpm), p_c is the pressure (bar), T_c is the temperature (K), $R=8.33$ J/mol K is the gas constant; $\chi_{C_8H_{18}}$ and χ_{O_2} are the fuel and oxygen mole concentrations in percentage (%) respectively; and $(\chi_{O_2}/\chi_{C_8H_{18}})_s$ is the air-to-fuel ratio under stoichiometric condition. The constant 1.09 multiplying to T_c in Eq. (9) is a correction from the original model in Ref. [13] that accounts for the difference between iso-octane and gasoline based

on the experimental evidence in Refs. [8] and [18]. The composition terms $\chi_{C_8H_{18}}$ and χ_{O_2} are derived from Sec. 2 based on the variations on the controllable engine parameters λ and α via changing fuel and RBL with particular experimental engine.

Using the same principle as above for Eq. (8), it is shown in Ref. [12] that the combustion timing is captured without accounting for concentrations in the Arrhenius integral. A single scaling constant replacing the composition terms is sufficient to match all the experimental data covering a wide range of operating conditions at different fueling levels and different EGR levels. The model in Ref. [12] is denoted by the subscript PT indicating its inclusion of pressure and temperature effects and lack of composition effect,

$$AR_{PT}(\theta) = \int_{\theta_{IVC}}^{\theta_{SOC}} A p_c^n(\vartheta) \exp\left(-\frac{E_a}{RT_c(\vartheta)}\right) d\vartheta \quad (10)$$

with $A=0.4167$, $E_a=51510$ J/mol, $n=1.367$, and $R=8.33$ J/mol K is the gas constant. The parameters A , E_a , and n are determined using a standard nonlinear optimization routine (constr.m from MATLAB) that minimizes the error between θ_{SOC} , modeled through Eq. (10), and the experimentally determined crank angle of 1% fuel burned θ_{CA01} for all the experimental data introduced in Sec. 2.

Before comparing the two realizations AR_{PTC} in Eq. (9) and AR_{PT} in Eq. (10), the cylinder pressure and temperature histories are substituted in Eq. (9) and (10) by their calculated values based on the polytropic compression principle and their values at IVC. During compression, the cylinder pressure and temperature values are calculated using a polytropic compression from IVC to SOC, $p_c = p_{IVC} v_{IVC}^{n_c}$, and $T_c = T_{IVC} v_{IVC}^{n_c-1}$ with coefficient $n_c=1.3$ and the volumetric ratio $v_{IVC}(\vartheta) = V_c(\vartheta_{IVC})/V_c(\vartheta)$, where the cylinder volume at crank angle ϑ , $V_c(\vartheta)$, is a function of the CR [22]:

$$V_c(\vartheta) = V_d \left[\frac{1}{CR-1} + \frac{1}{2} (R_c + 1 - \cos(\vartheta) - \sqrt{R_c^2 - \sin^2(\vartheta)}) \right] \quad (11)$$

with V_d the displaced volume (m^3) and R_c the ratio of connecting rod length to crank radius.

Figure 2 shows a comparison of the experimental data and θ_{SOC} predicted by the Arrhenius integrals AR_{PTC} in Eq. (9) and AR_{PT} in Eq. (10). Both models overpredict SOC at low fuel and high RBL operating points in Test A and similarly underpredict SOC at low RBL values in Test B. The mismatch at some operating points between θ_{SOC} predicted by AR_{PTC} in Eq. (9) and the data may result from the difference between iso-octane and gasoline. On the other hand, the good agreement between the AR_{PT} model and the data indicates that composition could possibly be ignored without degrading the prediction of θ_{SOC} . The same conclusion is reached by Najt and Foster [5] and Zhao et al. [11]. Before concluding that temperature is the dominant factor for the ignition timing, we shall verify that the sensitivity of SOC to composition is small even for the AR_{PTC} model in Eq. (9) that includes composition.

4 Thermal Dominance for Combustion Initiation

To explore further which variables dominate the autoignition process, we analyze the sensitivity of a parametrized Arrhenius integral for iso-octane derived from the ignition delay formula in Eq. (9). The sensitivity of the Arrhenius integral in Eq. (9) with respect to parameter X (p_{IVC} , T_{IVC} , $\chi_{C_8H_{18}}$, χ_{O_2} , CR, and θ_{IVC}) is

$$S_X = \frac{X}{AR_{PTC}} \left(\frac{\partial AR_{PTC}}{\partial X} \right) \times 100\% \quad (12)$$

The sensitivity calculation provides local information and depends on the operating conditions. Note first that since the AR_{PTC} is a nonlinear function of the variables of interest, the sensitivity needs to be evaluated at all operating points. The sensitivity of the

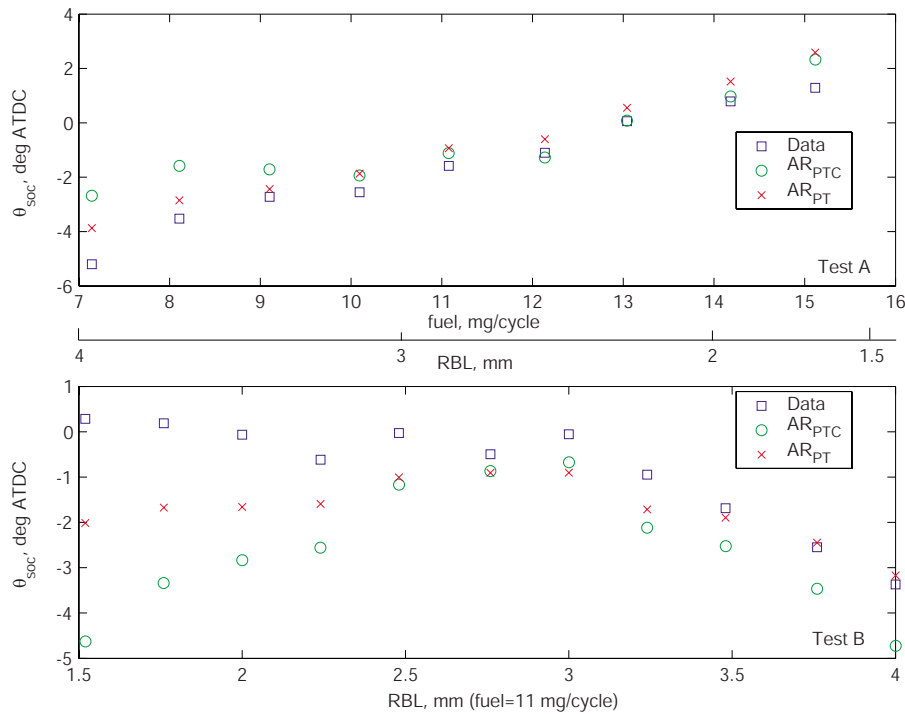


Fig. 2 Start of combustion: Test A and Test B for the Arrhenius integral with and without composition terms

Table 2 The sensitivity of the Arrhenius integral ($AR_{X_{He}}$) with respect to p_{IVC} , T_{IVC} , $\chi_{C_8H_{18}}$, χ_{O_2} , CR, and θ_{IVC}

	$S_{p_{IVC}}$	$S_{T_{IVC}}$	$S_{\chi_{C_8H_{18}}}$	$S_{\chi_{O_2}}$	S_{CR}	$S_{\theta_{IVC}}$
Test A	105%	1590–1680%	77%	64%	531–593%	–715% to –685%
Test B	105%	1614–1637%	77%	64%	538–566%	–701% to –694%

Arrhenius integral in Eq. (9) is calculated at all the operating points from Test A and Test B, and the results are summarized in Table 2. When a range of values is reported in a cell in Table 2, it indicates variations in the associate sensitivity of various operating points. When the variation is very small, one value is reported. As can be seen by the large numbers in Table 2, temperature T_{IVC} is the dominant factor in determining the combustion timing. The dominance of the temperature effect is also revealed by the experimental data in Fig. 2. Specifically, as discussed in Sec. 2, an increase in RBL results in a higher temperature T_{IVC} and reduced concentrations ($\chi_{C_8H_{18}}$ and χ_{O_2}). Test data in Fig. 2 (square symbols) show that as RBL increases, SOC advances, which can be solely predicted by the increase in T_{IVC} . Note also that pressure p_{IVC} is more important than the fuel and oxygen concentration, indicating the importance of the manifold filling dynamics and flow patterns for the autoignition timing. CR and IVC timing θ_{IVC} also have a strong influence on the ignition timing, indicating the possibility of using IVC timing as an actuator for ignition timing control as proposed in Ref. [23].

5 Conclusion

In this sensitivity study, the charge temperature effect and dilution effect on the ignition timing in a wide range of operating conditions of a port-injection gasoline HCCI engine are explored. By conducting sensitivity analysis of an ignition timing model developed in Ref. [13], we find that the SOC timing depends much more on temperature than on composition. There may exist,

however, conditions when composition changes more than temperature does, such as when there is high heat loss in the cylinder and cylinder temperature does not change much despite increased exhaust dilution [24]. It is not clear at this point if such extreme heat transfer conditions will benefit an automotive engine application. Thus, we conclude that the composition effects can be eliminated from a control-oriented model for ignition timing to enable easy calibration in a port-injection gasoline HCCI engine.

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