ABSTRACT
In order to aid in the design and development of small-scale internal combustion (IC) engines, the burning speed and structure of flames ignited in small, constant volume chambers have been observed and modeled. Experiments were performed in a scaled combustion chamber with similar geometry to a Wankel engine application to determine the operating conditions necessary for combustion to occur on the small scale. The chamber has a quartz window for visual observation and a pressure transducer to measure the pressure rise. A one-dimensional, laminar quench model using a one-step global reaction mechanism was developed to simulate the experimental results. High-speed (up to 2000 frames per second) schlieren video was used to visualize combustion events. These images were compared to predictions of a 2-D numerical model of the flame propagation. These models further clarify the transition from ignition kernel to combustion wave and the flow fields inside the chamber. The results from these experiments and modeling will assist in the development of small-scale IC engines.
INTRODUCTION
This project is one part of the rotary engine development project at Berkeley [1]. The goal of the project is to develop a device for portable power generation in the range of 10-100 watts using liquid fuels. If the high specific energy of liquid hydrocarbon fuels can be converted at high efficiency, coupling an engine to a small generator would achieve a higher specific energy than batteries of comparable size and weight. However, constraints to combustion at small scales require special approaches to sustain combustion.

The objective of this study is to understand the limits of combustion when the size is small and the ignition energy is limited. Three parameters are being investigated. The pressure is changed to simulate conditions in the engine after compression. The temperature is varied to reduce heat losses and increase the reaction rate. The ignition energy is reduced to minimize the amount of parasitic power drawn from the engine, while still igniting the mixture.

In order to understand the combustion process that occurs in engines of this scale, the ignition event has been examined separately from the rest of the engine operation. In this way, the effects of other variables on combustion during engine operation are removed, such as sealing, compression ratio, spark timing, oil contamination, etc. As a first step, the geometry of a 1.0 kW Wankel engine has been studied. This engine has a displacement of 5.0 cc, which is over ten times larger than the Berkeley engine.

A common piece of diagnostic equipment used during engine operation is a pressure transducer, which is problematic at these small sizes since the size of the dead volume is of the same order of magnitude as the combustion chamber. This has the effect of reducing the compression ratio, and therefore the maximum pressure, in the engine. Optical techniques do not have this problem since they do not require any dead space inside the test section. Furthermore, the planar nature of the Wankel engine is conducive to optical techniques, however the small volume reduces optical path lengths and makes quantitative measurements difficult.

Visualization of density gradients is a powerful tool to obtain a better understanding of combustion. Our primary goal when using the schlieren technique [2] is to measure the propagation speed of the flame, as well as to visualize ignition and flame propagation, inside our small chambers.

In addition, an analytical and numerical modeling effort has been part of this work to gain a more fundamental understanding of the experimental data. A one dimensional, laminar quench model using a one-step global reaction mechanism was created to initially validate the experimental results involving the boundary region of ignition and non-ignition in the chamber.

A 2-D numerical combustion model with eight-step chemical reactions for hydrogen-air was also developed as a first step toward a model that simulates the schlieren images of
flame propagation. It has also been used to determine the boundary conditions for ignition for hydrogen-air mixtures.

EXPERIMENTAL SET UP
A static combustion chamber was developed to determine a flammability region over a range of temperatures and pressures. Then a similar chamber was used with a schlieren optical apparatus to obtain high-speed video of combustion under the same conditions.

The static combustion chamber was designed to duplicate the geometry of the Wankel engine at top dead center (TDC), the minimum chamber volume at which combustion is initiated. Figure 1 shows side and cross-sectional views of the Wankel engine at TDC and our static test chamber. As an initial testing device, the curved surfaces have been approximated as planes, keeping the overall dimensions the same. The dimensions of the static chamber are 22 mm x 7.9 mm x 1.6 mm with a volume of 278 mm$^3$.

Figure 1: Side and cross-sectional views of rotary engine and static test chamber

Figure 2: Image of test chamber for schlieren imaging, including strip heater
Ignition tests were performed with a stoichiometric mixture of butane and air over a range of initial pressures from 1 atm to 6 atm and at four initial temperatures (25°C, 50°C, 100°C, 150°C). Two ignition energy levels were tested, 40 mJ and 400 mJ.

The auxiliary equipment included a 2.25 L mixing chamber (Whitey 304L SS DOT-3A 1800) that contained the fuel and air at a specific stoichiometry. Two solenoid valves (Asco 8225B-006V) and a 0-200 PSIG Omega pressure transducer (model # PX176-200S5V) were used to fill the chamber to a set pressure. A 3” x 1” 50W strip heater and a temperature controller (Watlow model S1A3JP1 and 96A1-CKAR) controlled the temperature. Either a 100 or 1000 µF capacitor was charged to 28.3 volts and discharged through both an ignition coil with a 100:1 turns ratio (MSD Blaster part # 8223) and a custom tungsten electrode to ignite the mixture. It should be noted that the energy measured is the energy that is discharged from the capacitor, not what is delivered to the fuel-air mixture, as there are certain losses in the ignition system. For high data rate pressure measurements, an aluminum plate and a Kistler 601B pressure transducer was mounted with a Type 222P needle adaptor over the combustion chamber. For visual observations, the aluminum plate was replaced with a quartz plate (See Figure 3).

The test procedure was to set the chamber to a given temperature and then fill the chamber with a fuel-air mixture to a set pressure. The mixture was allowed to thermally equilibrate for ten seconds and then an attempt was made to ignite the mixture by discharging a capacitor with a fixed amount of stored energy.

For the schlieren testing, a plane mirror is mounted directly on the rear side of the chamber. This mirror folds the light back through the test section to avoid optical obstruction by the igniter and increases the total test section light path length, thereby increasing resolution (see Figure 2). The schlieren system consists of a xenon light source (35W), a collimating mirror, a flat mirror (in the rear of the combustion chamber), a beam splitter, a slide for colorization, and a high-speed camera (Kodak EktaPro HG Imager, Model 2000). Using the high-speed camera, pictures can be taken at up to 2000 frames per second with an exposure time of 483 µs. Pictures are stored in TIFF format and downloaded to the local hard drive.
Figure 3: Apparatus for ignition testing

Figure 4: Apparatus for schlieren visualization
EXPERIMENTAL RESULTS
To measure whether or not ignition has occurred in our static combustion chamber, the capacitor is discharged through the electrode into a mixture at a known temperature, pressure and stoichiometry. When using the higher ignition energy of 400 mJ, ignition was detected for all the initial pressures and temperatures tested, including the lowest setting of 25°C and 1 atm. An engine using this much ignition energy operating at 10,000 RPM would require 67 watts of continuous power. Since this energy must ultimately come from the power generated by the engine, 400 mJ is impractical. Using a lower energy of 40 mJ, ignition was observed only under certain conditions.

Representative pressure traces for 25°C with a 40 mJ spark can be seen in Figure 5. At the lower pressure of 1 atm, no pressure pulse was detected after the spark. At higher pressures, a pressure pulse is detected. As the initial pressure is increased, the pressure difference also increases. An initial pressure of 3 atm resulted in a peak pressure difference of 11 atm and a starting pressure of 5 atm lead to a 31 atm peak pressure difference.

The effect of initial pressure on ignition for a 40 mJ discharge at 25°C can be seen in Figure 6. Below 1.8 atmospheres, no pressure pulse was detected. A small rise in pressure was detected between 1.8 and 2.3 atm. Above 2.3 atm, the pressure rise steadily increased. These values were compared to the pressure rise predicted by STANJAN under constant volume and internal energy conditions (Figure 7). The measured pressure differences were lower than predicted at low initial pressures, but reached the predicted values at initial pressures of 6 atm. This can be attributed to the incomplete combustion at low pressures due to partial quenching on the side walls.

By continuing this test at several temperatures and determining the initial pressure where ignition occurs, a map of the ignition region as a function of pressure and temperature can be generated. Ignition is assumed to occur when there is any detectable pressure rise. Such a map for stoichiometric butane-air mixtures using an ignition energy of 40 mJ can be seen in Figure 8.
Figure 6: Effect of pressure on pressure difference

Figure 7: Comparison of experimental data and STANJAN prediction

Figure 8: Pressure-Temperature boundary for ignition in 1.6 mm chamber with butane-air at $\Phi = 1.0$ and 40 mJ ignition energy.
Schlieren images were collected for stoichiometric butane-air mixtures with varying initial pressure and temperature and an ignition energy of 400 mJ. The initial conditions with which the schlieren visualization was carried are tabulated in Table 1.

Schlieren images taken for the condition of 4 atm and 100°C are shown sequentially in Figure 9. Red color intensities of the original image (as the light is passed through the color slide shown in Figure 4) were extracted and converted into gray scale to emphasize the flame front propagating in the chamber. From these sequential images, we obtained a flame propagation speed of approximately 4 meters per second, which is 11 times faster than laminar flame speed of stoichiometric butane, 34 cm/s at 4 atm. This higher speed will be discussed in the Two-Dimensional Flame Propagation Modeling section.

When using 400 mJ of ignition energy, flame propagation was observed inside the test section for all test conditions studied during these experiments, including 1 atm and 25°C. Note that the narrow cross section of our test chamber is 1.6 mm, half of the quenching distance, 3.0 mm, of a stoichiometric butane-air mixture at 1 atm and 25°C quoted in the literature. More work is ongoing to determine the impact of critical chamber dimension on ignition, but these results clearly indicate that combustion can be controlled at the small scale and are not a fundamental combustion limit.

It is also considered that under lower initial temperature and pressure regions (lower-left in Figure 8) the combustion process was incomplete and did not show a significant pressure rise. These visual observations were confirmed by the pressure measurements (as shown in Figures 5 through 7) and indicate that weaker initial combustion fronts are strongly affected by the losses to the chamber walls.

Table 1: Schlieren experimental conditions: conditions for Figure 8 are in bold

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<th>Pressure (atm)</th>
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MODELING RESULTS

One-Dimensional Quenching Regime Model

A one-dimensional, laminar quench model using a one-step global reaction mechanism was developed to verify the experimental ignition results. Since the chamber is much longer and wider than it is thick, a 1-D analysis can be used. The model assumes that quenching occurs when the ratio of heat being generated to the heat being lost is less than 1 [1]. The heat generated is due to combustion, and the heat lost is assumed to be only from conduction.

\[
q_{\text{gen}}^{''} = \frac{\dot{m} c_p \Delta T_f}{A} = \rho V c_p \Delta T_f
\]

\[
q_{\text{cond}}^{''} = \frac{k}{d_q} \frac{\Delta T_c}{d_q}
\]

\(d_q\) is the distance between the flame and the wall (See Figure 10).
\( \Delta T_f \) is the temperature rise due to combustion.  \( \Delta T_c \) is the temperature difference between the flame and the wall.  Assuming \( \frac{\Delta T_f}{\Delta T_c} \) is constant, and substituting \( \alpha \) for \( \frac{\rho c_p}{k} \),

\[
\frac{d_q V_l}{\alpha} = \text{constant} = Pe
\]

where \( Pe \) is the Peclet number.

The limiting chamber depth for quenching is found to be:

\[
d = 2 d_q = \frac{2 Pe \alpha}{V_L}
\]

For this model a simplified laminar flame model similar to that of Mallard and LeChatlier is used [1].

\[
V_L = \left[ \frac{\left( \frac{\alpha \bar{r}_f}{\bars{n}_f} \frac{1}{2} \left( T_f - T_{ig} \right) \right)}{T_{ig} - T_o} \right]^{\frac{1}{2}}
\]

\( T_o \) is the reactant and wall temperature. \( T_{ig} \) is the ignition temperature taken from [1] and is assumed to be the same for all conditions.  The adiabatic flame temperature, \( T_f \), is calculated with STANJAN at 1atm and 25°C at several stoichiometric ratios.  Due to the inherent limitations of the model, \( T_f \) is assumed not to change with pressure or initial temperature.  The reaction rate, \( \bar{r}_f \), is approximated by the following one-step global reaction mechanism with the temperature taken as the average of the reactant temperature and the adiabatic flame temperature [1].

\[
\bar{r}_f = -A \exp\left( -E / RT \right) \left[ \text{fuel} \right]^a \left[ O_2 \right]^b
\]

where the global reaction constants of \( A = 7.4E11 \), \( E = 30000 \) cal/kgmol, \( a = 0.15 \), and \( b = 1.6 \) are taken from [3].
Since it is not known a priori what the Peclet number should be, the model needs to be calibrated with experimental data. As a starting point, published quenching data is used [2]. With one data point of $d_q = 3.05$ mm for butane at 1.0 atm, 25°C, and $\Phi = 1.0$, extrapolations can be made to other temperatures, fuel-air ratios, pressures and chamber dimensions. The excel model that uses these equations has been set up to mimic the inputs and outputs of an experiment. The user inputs are: 1) fuel 2) stoichiometry 3) distance and 4) temperature. The output is the pressure and flame speed. In order to solve for the pressure, the excel “solver” operation must be performed which minimizes the squared difference between the calculated quench distance and the input distance.

Results of this model for a stoichiometric butane-air mixture in a 1.6 mm channel can be seen in Figure 8. The model agrees fairly well for the case where the ignition energy is 40 mJ.

Two-Dimensional Ignition Regime Model

A two dimensional numerical model has been created to understand both the predictions of the 1-D model and the experimental results. The physical model is based on a zero-Mach-number of the compressible conservation equations [6]. In the model, the pressure field is decomposed into a spatially uniform component $P_0$ and a hydrodynamic component $p(x,t)$ which varies both in space and time. Attention is restricted here to open domains; i.e., the thermodynamic pressure $P_0$ is constant in time as well. The present model assumes a two dimensional flow, zero bulk viscosity, and a detailed chemical reaction mechanism that involves $N$ species and eight elementary reactions. Soret and Dufour effects, radiant heat transfer are ignored. The mixture is assumed to obey the perfect gas law, with individual species molecular weights, specific heats and enthalpies of formation, using Fickian binary mass diffusion.

Numerical calculations to find the conditions necessary for ignition have been done with 257x51 grid points as shown in upper half of Figure 11, which has dimensions of 0.8 mm in height and 10 mm in length and utilizes symmetry conditions to reduce the effective numerical grid area. The dimensions of the calculation domain are the same size as the narrow cross section of the chamber used in the experiments. During the calculations, thermal boundary conditions were prescribed as constant temperature on top and adiabatic on the other walls to fit the experiment. An isothermal wall was used as the upper boundary since the wall temperature in the experiment was controlled to a fixed value by a heater (see Figure 2). Velocity boundaries are as follows: left and bottom wall were set to symmetric, top wall was set to non-slip, and the right wall was open to ambient pressure. A hydrogen and air mixture was used for fuel at a fixed stoichiometry of 1.0. Each calculation was done by varying the ambient pressure from one to two atmospheres and wall temperatures from -73 °C to 127 °C to determine whether the mixture would ignite or not. The ignition source for these calculations was a hot temperature spot in the center of channel with maximum temperature fixed at 1227 °C.

From the results shown in Figure 12, one can see the boundary where ignition would occur. The line goes through the point at a pressure of 1.2 atm and temperature of
-73°C to the point at a pressure of 1.0 atm and temperature of 127°C. This graph shows that when the hydrogen is used for fuel and burned at stoichiometric conditions, it will always ignite in an engine of the present size and operating conditions. The trend is similar to the results of one dimensional model and experiments. Experiments with hydrogen and air are on going to corroborate findings.

Figure 11: Modeled quarter section of combustion chamber

![Iso Thermal Wall](image)

![Symmetric Wall Condition](image)

![Adiabatic non-slip wall](image)

![Symmetric Wall](image)

![Open to Ambient](image)

Figure 12: Numerically modeled ignition boundary for stoichimetric H₂-air mixture

![Ignited vs. Not Ignited Points](image)
Two-Dimensional Flame Propagation Modeling

Further numerical research was done to investigate the flame propagation speed. In these calculations, a 4mm x 10mm section with 74x28 nodes was used (see lower half of Figure 11). This gives a constant grid length of 0.3mm, half of the flame thickness of a stoichiometric hydrogen-air mixture [7]. The size of calculation domain is the same as that of wide cross section of chamber, which is shown in previous schlieren images. Pressure and velocity boundary conditions are the same as the former calculation except for right wall. Instead of being fully open, the right wall is closed except for a 1mm wide outlet at the bottom which is open to ambient pressure.

The reason an open boundary is prescribed at the right wall is because it is suspected that the chamber is not fully closed as discussed before in schlieren experiment section, but is instead open to the pressure transducer dead volume next to the test section. Adiabatic thermal boundary conditions were applied to all walls. Characteristic time for the thermal diffusion into wall, 10µs, is larger than that for chemical, 5 µs so that the impact of heat loss to the surrounding walls is estimated to be relatively small for hydrogen fuels. Care must be taken, however, to extend these model results for other chemical and geometric effects.

The same ignition procedure as the previous calculation, i.e., hot spot with maximum temperature 1227°C, is also used. Initial temperature other than ignition region was set to 127°C and initial pressure was 1.0 atm.

When the propagation speed was measured in the same manner as the schlieren experiments, the propagation speed was 8 m/s, which is approximately 4 times faster than the planar laminar flame propagation speed, 2.0 m/s at 2 atm [8].

As noted in the schlieren experimental section, the measured flame speed for butane-air was 4 m/s, much higher than the laminar flame speed of 34 cm/s. It is considered that the higher flame propagation speed may be attributed to an outward flow velocity that convects the flame surface to either end. A flow velocity of about 5 m/s is obtained for hydrogen-air from this 2-D calculation. The sum of the flow velocity from the calculation and the flame propagation speed from literature gives us the flame speed of 7.0 meters per second, which agrees with the propagation speed from the results. More work is ongoing and expected to resolve the discrepancy in flame speed measurements.

The existence of leakage flow is strongly confirmed when the flame shape feature from modeling and schlieren images were compared. This comparison can be found in Figure 14, which shows the flame protruding in the center just before it reaches the end of the chamber. From these figures, we conclude that the leakage flow to the dead volume exists and affects the flame propagation velocity from fixed chamber coordinates. Combined with the accelerated burning speed of 2 m/s due to elevated pressure, the net propagation speed, 7 m/s, shows good agreement with the numerically observed flame speed of 8 m/s.
Figure 13: Modeled flame propagation for stoichiometric hydrogen-air

Figure 14: Comparison between modeled flame shape with schlieren images
CONCLUSIONS AND FUTURE WORK
An apparatus has been constructed to measure the ignition boundary region in small combustion chambers with a similar geometry to that of a 1kW rotary engine. With this apparatus, the ignition boundary for butane and air as a function of pressure and temperature has been determined. The experimental data agrees with a one-dimensional quench model under certain ignition energy conditions.

Experimentally measured flame speeds were up to eleven times higher than the laminar flame speed cited in the literature. It is postulated that there exists a significant outward flow which is causing this observed discrepancy. Numerical results also predict a higher flame speed under similar conditions.

Future work will include testing of smaller chambers to further understand the effects of high surface area to volume ratio chambers on combustion. Increased spatial resolution of the optical system, coupled with the numerical results will help ascertain the impact of wall quenching on pressure rise in small combustion volumes. The effect of flowing mixtures will also be determined in order to more closely mimic the conditions during engine operation.

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REFERENCES


