Milestone Report #2: Direct Evaporator Leak and Flammability Analysis

*Modifications and Optimization of
the Organic Rankine Cycle to
Improve the Recovery of Waste
Heat*

Donna Post Guillen

September 2013

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ABSTRACT

The direct evaporator is a simplified heat exchange system for an Organic Rankine Cycle (ORC) that generates electricity from a gas turbine exhaust stream. Typically, the heat of the exhaust stream is transferred indirectly to the ORC by means of an intermediate thermal oil loop. The goal of this project is to design a direct evaporator where the working fluid is evaporated in the exhaust gas heat exchanger. By eliminating one of the heat exchangers and the intermediate oil loop, the overall ORC system cost can be reduced by approximately 15%. However, placing a heat exchanger operating with a flammable hydrocarbon working fluid directly in the hot exhaust gas stream presents potential safety risks. The analyses presented in this report assess the flammability of the selected working fluid in the hot exhaust gas stream stemming from a potential leak in the evaporator. Ignition delay time for cyclopentane at temperatures and pressure corresponding to direct evaporator operation was obtained for several equivalence ratios. Results of a computational fluid dynamic analysis of a pinhole leak scenario are given.

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ACRONYMS

AFT	Adiabatic Flame Temperature
CFD	Computational Fluid Dynamics
DE	Direct Evaporator
EBU	Eddy Breakup
IDT	Ignition Delay Time
IQT	Ignition Quality Tester
LES	Large-Eddy Simulation
ORC	Organic Rankine Cycle
RANS	Reynolds-Averaged Navier Stokes
TEG	Turbine Exhaust Gas

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1. INTRODUCTION

Turbines and engines used in industrial applications produce copious amounts of waste heat. If even a fraction of this waste heat could be economically converted to useful electricity, it would have a tangible and very positive impact on the economic health, energy consumption, and carbon emissions in the U.S. manufacturing sector. Land-based gas turbines are used in a broad range of applications to produce both shaft and electrical power. Most commonly known for generating electricity as either peaking units or as base load units, these turbines are also used to directly drive pumps, compressors, or other machinery requiring shaft power. Simple cycle gas turbines have the advantage of a short startup time relative to coal-fired and nuclear units, however, they incur a significant penalty on their efficiency. Large frame gas turbines usually are combined with bottoming steam-based Rankine cycles to increase the overall efficiency of the system and thereby improve their cost performance. Small-frame gas turbines with exhaust temperatures around 773 K could, in principle, benefit from steam bottoming cycles, but rarely use them in practice because the fixed overhead costs of the steam system are too great. Particularly for base-load, small-frame gas turbines, like those used in pipeline applications, an increase in efficiency is highly desirable. Organic Rankine Cycles (ORCs), as depicted in Figure 1, are a viable option to recover the exhaust waste heat and use the ambient air as a heat sink. The turbine exhaust gas (TEG) is available at temperatures between 673 and 823 K.

Figure 1. Typical layout for an ORC in the role of a bottoming cycle for a gas turbine.

The ORC is a vapor power cycle that operates using the same principles as the steam Rankine cycle, except that a fluid with a lower boiling point (and higher molecular mass) is used. A hydrocarbon or refrigerant working fluid is evaporated, instead of boiling water to create steam, to run through a turbine to generate electricity. This enables the operation of the cycle at much lower temperatures than a steam Rankine cycle, allowing the ORC to use the energy from low temperature waste heat sources to produce electricity.

The Rankine cycle contains four main components: evaporator or boiler, turbine or expander, condenser, and pump. Depending on the working fluid, a recuperator may be advantageous, depending on the shape of the vapor dome. A positive slope of the saturated vapor curve on the temperature-entropy diagram precludes the need to superheat the working fluid to avoid condensation in the turbine. The heat source in ORC systems is coupled to a heat exchanger to evaporate the working fluid before it is expanded in the turbine. The efficiency of an ORC depends both on the initial temperature of the waste heat and the level of irreversibility introduced as that heat is transferred to the cycle fluid, then from the cycle fluid to the heat sink.

In low temperature applications like geothermal power, hot water or steam can be coupled directly to the ORC evaporator. However, in high temperature applications like gas turbines, the hot exhaust gas may cause decomposition of the hydrocarbon-based working fluid, making safety a major concern because of the high flammability of these working fluids. The exhaust gas heat exchanger is traditionally isolated from the evaporator by an intermediate oil loop to transport the heat between the heat source and the working fluid. These systems offer only marginal economic benefits since the secondary loop incurs additional costs for each unit, increases the opportunity for component failure, and reduces the conversion efficiency of the system.

To overcome these issues, our project team is working to develop an efficient, cost-effective ORC system using “direct evaporator” technology. The goal of this project is to design a direct evaporator wherein the working fluid is evaporated in the exhaust gas heat exchanger. By eliminating one of the heat exchangers and the intermediate oil loop, the overall ORC system cost can be reduced by approximately 15%. However, placing a heat exchanger operating with a flammable hydrocarbon in the hot exhaust gas stream presents potential safety risks. The analyses presented in this report assess the flammability of the selected working fluid in the hot exhaust gas stream stemming from a pinhole leak in a finned heat exchanger tube.

2. DIRECT EVAPORATOR DESIGN

The direct evaporator design shown in Figure 2 includes three sections of heat exchange tube banks with working fluid inside, performing the function of an evaporator, superheater, and economizer suspended in a rectangular duct. The configuration is similar to a conventional heat recovery steam generator unit, except there are no duct burners. There are two tube rows in the evaporator, two in the superheater, and 24 in the economizer, respectively, for a total of 28 rows with 60 tubes in each row. The direct evaporator is designed to mate with a General Electric small-frame gas turbine, where the hot TEG flows across the tube bundles. The vaporized working fluid is supplied to a turbine to generate additional power.

The working fluid selected for this application, cyclopentane, flows in a counterflow arrangement through the tube bundle. In the protective staging concept employed by the DE design, the hot TEG enters the heat exchanger and flows past the evaporator, superheater, and economizer, in that order. This arrangement limits the maximum temperature of the working fluid to prevent degradation. The rationale for the selection of cyclopentane as the working fluid was presented in detail in Milestone Report #1 (2010), “Design and Modeling of Direct Evaporator.”

Figure 2. Direct evaporator design.

3. IGNITION MECHANISMS

As shown in Figure 3, oxygen, heat, and fuel are the three elements necessary for a fire to occur. If the temperature is high enough, an ignition source is not necessary to initiate combustion. Autoignition occurs when sufficient self-heating by chemical reactions takes place to accelerate the rates of reactions to produce full-scale combustion. Combustion is the sequence of exothermic chemical reactions that occurs between a fuel and an oxidant accompanied by the production of heat and conversion of chemical species. Combustion feeds a fire with heat, enabling the process to continue.

Figure 3. Fire triangle (courtesy of Wikimedia Commons).

In the proposed ORC design, oxygen, heat, and fuel (cyclopentane) are present, creating the potential for a fire in the direct evaporator. The autoignition temperature of cyclopentane is 634 K (360.9°C), substantially below the inlet exhaust gas temperature of 803K. Flammability limits at atmospheric pressure are between 1.4 and 9.4% (Chevron-Phillips, 2009). The low lower flammability limit is indicative of a weak bond that scissions and breaks in the ring. It also indicates that radicals are formed, which are not terminated quickly. Cyclopentane is a cycloalkane classified as a DOT Hazard Class flammable liquid (per 49 CFR 172.1 and 49 CFR 173) and OSHA Classification (29 CFR 1910.1200) with a flash point of 236 K (Gallant and Yaws, 1993).

Because of the large pressure difference between the working fluid inside the heat exchanger tube (44 bar) and atmospheric pressure, the leaked fluid is assumed to instantly flash to vapor since the boiling point of cyclopentane at atmospheric pressure is quite low (322K) (Gallant and Yaws, 1993). As the working fluid escapes from a high pressure to atmospheric pressure, the vapor is released into the TEG. Since the fuel source is introduced in the form of a jet, the occurring thermochemical phenomena correspond to non-premixed combustion conditions. The heat release of the cyclopentane by autoignition serves as the ignition source for further combustion. Complete combustion of cyclopentane (in the absence of other gases besides oxygen) is represented by the following equation:

The reaction rate depends on the mean species concentration of the mixture and the local mean temperature. The concentration field and the progress of chemical reaction are affected by the topology of the turbulent flow field (Bergeron and Hallett, 1989).

Ignition processes are usually very complex and involve many intricate physical and chemical steps (Agarwal and Assanis, 2001). These steps take a finite amount of time and the period between the start of injection and the start of combustion is referred to as *ignition delay time*. The ignition delay time is a latent period in the combustion process, during which the temperature remains nearly constant (Golovitchev and Chomiak, 1998). The delay time is comprised of a physical delay and a chemical delay component. Physical delay is caused by the finite rate of mixing of injected cyclopentane with hot exhaust gas and is the time needed for the flammable gas mixture to reach the autoignition temperature. The chemical delay is caused by the precombustion reactions of the combustible gas mixture that lead to autoignition. For hydrocarbon and air/oxygen mixtures, this induction period before the reaction accelerates can vary between seconds and hours (Jost, 1946). At low temperatures, fuel-air mixtures react chemically and produce very weak flames (cool flames). The fuel and oxygen molecules have little energy and do not react vigorously; therefore, the reaction never proceeds to complete combustion. Instead, the molecules break down and recombine to produce a variety of stable chemical compounds. If the rates at which the heat liberated from breaking and reforming of the chemical bonds exceeds the rate at which heat is lost to the surroundings, cool flames develop, and the mixture autoignites.

In the heat exchanger, both the physical and chemical processes are occurring simultaneously and cannot be decoupled. Therefore, the actual autoignition delay time in a flowing system is difficult to determine, as it will be affected by the following steps (Goy, Moran, and Thomas, 2001):

1. Time required for fuel and TEG to mix
2. Time for the fuel temperature to rise to that of the TEG
3. Chemical-kinetic time for the autoignition reactions to initiate.

No published data were found on autoignition delay time for cyclopentane at the temperatures and pressures of interest. However, the literature clearly indicates that autoignition delay time increases with decreasing temperature.

The literature shows that a detailed chemistry model is essential for the prediction of ignition delay because the minimum ignition energy and induction time cannot be well predicted by simplified

chemistry. The complex nature of the physicochemical processes leading to ignition makes the numerical solution of detailed chemical kinetics coupled with the flow essential for any kind of quantitative prediction. In addition, mixing and ignition are three-dimensional, transient phenomena that require a coupling of the detailed chemical-kinetic mechanism with a multidimensional flow simulation. Ignoring the injection and flow processes can lead to predicted values of ignition delay that are lower by more than an order of magnitude compared to experimental values (Agarwal and Assanis, 2001). Measured autoignition delay times and chemical-kinetic mechanisms describing autoignition and combustion of cyclopentane at the conditions present in the direct evaporator were not found in the open literature.

4. AUTOIGNITION EXPERIMENTS

There is a lack of IDT data available in the public domain for cyclopentane covering the range of initial temperatures, pressures, and oxygen concentrations relevant to ORCs with DEs. Much of the data is either at too high of a temperature (>1000 K), at too low or too high of a pressure, or for dilute concentrations. Sirjean et al. (2007) published ignition delay times for cyclopentane in the temperature range from 1300 to 1800 K. The general trend displayed is that IDT increases with decreasing temperature up to two orders of magnitude over this temperature range. Daley et al. (2008) measured ignition delay times for cyclopentane-air mixtures in a shock tube at temperatures of 847 to 1379 K, pressures of 11 to 61 atm, and equivalence ratios (Φ) of 1.0, 0.5, and 0.25. Other published ignition delay data found are for relatively dilute mixtures of cyclopentane in argon (Sirjean et al., 2007; Orme et al., 2005). Sirjean et al. (2007) measured ignition delay in a shock tube for cyclopentane-oxygen-argon mixtures with fuel concentrations of 0.5 and 1.0%, respectively, and equivalence ratios of 0.5 to 2.0 (O_2 concentrations of 1.875% to 9%), temperatures from 1230 to 1840 K, and pressures from 7.3 to 9.5 atm. Orme et al. (2005) made similar shock tube ignition measurements for cyclopentane-oxygen-argon mixtures with a cyclopentane concentration of 1.0%, equivalence ratios of 0.577 to 2.0 (O_2 concentrations of 3.5% to 13%), temperatures from 1370 to 1820 K, and pressures near 1 atm. Shock tube results with mixtures of cyclopentane, cyclopentene, cyclopentadiene and dicyclopentadiene in argon with a fuel concentration of 1.0% and O_2 concentration of 13.0%, displayed very similar IDTs. The researchers concluded that it is the concentration of O_2 rather than the equivalence ratio that affects the IDT. Using a shock tube, Buda et al. (2005) measured IDTs of cyclopentane-oxygen-argon mixtures (0.5 or 1% of hydrocarbon, equivalence ratios from 0.5 to 2) at temperatures from 1230 to 1800 K and pressures from 7.3 to 9.5 atm. Reitzer and Lamb (1955) used a rapid compression machine to obtain IDTs for stoichiometric mixtures of cyclopentane and air over the range of temperatures from 803 to 1033 K and pressure from 2.3 to 3.25 MPa. Autoignition data were not found in the literature for cyclopentane at the conditions of interest (e.g., 13.3% O_2 environment at 803 K and atmospheric pressure).

4.1 Experimental Setup and Methods

A determination of the IDT for the actual ORC operating conditions was necessary in order to specify appropriate safety controls. Southwest Research Institute (SwRI, San Antonio, TX) was commissioned to perform ignition delay tests with cyclopentane. SwRI has extensive experience analyzing fuels with various techniques for many different manufacturers. The test procedure employed the same methods used in previous projects conducted at SwRI. A photograph of the Ignition Quality TestTM (IQTTM) Laboratory Model from Advanced Engine Technology Ltd. (Ottawa, Ontario, Canada) used to perform the testing is shown in Figure 4. Figure 5 illustrates the operation of the IQTTM apparatus. This test apparatus injects a small amount of fuel into a heated, temperature-controlled constant-volume chamber charged with compressed air. The 0.213 liter combustion chamber is surrounded by insulation. It is equipped with external electrical heating elements and pneumatically-actuated intake and exhaust valves. A heated, pneumatically-actuated fuel injection system with adjustable positive displacement pump, injector nozzle assembly, and sample reservoir provides the test fluid to the chamber. The coolant system has a liquid-to-air heat exchanger, filter, circulating pump, and flow control valves. A proximity sensor on the injection nozzle is used to record the start of injection. The fuel injection system is a Pintle-type,

single-hole nozzle with an air-driven fuel injection pump. The fuel injector for the IQT™ injects a fixed mass into the chamber. Each injection produces a single-shot, compression ignition combustion cycle. Ignition is sensed via temperature thermocouples, pressure gauges and sensors, an injector nozzle needle motion sensor, compressed gas pressure regulators, control valves, pneumatic actuator components, and solenoid valves.

Figure 4. IQT™ apparatus (courtesy of SwRI).

Figure 5. Schematic of IQT operation (from <http://www.stanhope-seta.co.uk/iqt.swf>).

Fuel is sprayed into an initially quiescent environment, where it immediately vaporizes. Ignition delay is measured using sensors that detect the start of fuel injection and the start of significant combustion for each cycle. The onset of ignition is sensed by the output of both pressure and heat flux gauges, which are fed into an oscilloscope. Ignition delay is measured from the start of needle lift to the chamber pressure recovery point. The pressure initially drops because of evaporation of the spray (Totten et al., 2003) as shown in Figure 6. Ignition is manifested by either a sudden rise in the plateau value of the traces or a

marked change in their slope. A complete sequence is comprised of 15 preliminary cycles and 32 additional test cycles. The ignition delay measured for the last 32 cycles is averaged. Per ASTM D6890 (2010), the system was calibrated using a chemical (n-heptane) with known IDT (Ciezki and Adomeit, 1993).

Figure 6. Trace for one run at $T = 803\text{ K}$, $\Phi = 1$.

As mentioned above, the ignition traces were manually recorded and post-processed to calculate ignition delay. This ignition delay is measured from the start of needle lift to the chamber pressure recovery point. The onset of ignition was sensed by the output of both pressure and heat flux gauges, fed into an oscilloscope. Its occurrence was manifested by either a sudden rise in the plateau value of the traces or a marked change in their slope.

4.2 Initial Results with Original Injector

This experiment involved testing cyclopentane in the IQTTM using ASTM D6890 (with exception to charge pressure and temperature) to determine ignition delay of the fuel at atmospheric pressure for normal air (~21% oxygen) and vitiated air (13.3% oxygen). The IQTTM is normally operated at 21.1 bar initial pressure and 835 K initial charge temperature. This testing required initial charge pressure and temperature of 1 bar, and 803 K respectively.

Using the IQTTM outside of its normal operating conditions caused a few issues. The standard software that runs the IQTTM system would not run with the low initial pressure, so the system had to be operated manually. Additionally, some of the ignition delay times were outside the recordable range for the software so the ignition traces had to be recorded on an oscilloscope and post-processed. Finally, the fuel injector for the IQTTM injects a fixed mass into the chamber, which now has roughly 21 times less mass leading to very rich conditions (0.95:1 air-fuel ratio or approximately 15 times too much fuel) and wall wetting and erratic ignition due to low charge density. To correct the air-fuel ratio for each combustion gas, or more specifically, the oxygen-to-fuel ratio, the injector pump was removed and adjusted to allow for lower injected mass. The injector and pump assembly were then calibrated by injecting 100 shots into a container and weighed to determine the mass per injection. This process was repeated until the desired fuel mass for stoichiometric combustion was achieved and then repeated three

times to determine repeatability. It was determined that 0.004 and 0.0063 grams of fuel would be needed to achieve stoichiometric combustion for the 13.3% and 21% O₂ combustion gases respectively.

The resulting ignition delays from the 13.3% and 21% O₂ runs varied greatly within the 32 run test. The average ignition delay and standard deviation were almost the same value for the atmospheric pressure tests. The ignition delay times varied from 3 ms to 90 ms for this testing. Table 1 provides the results for the two conditions as mentioned before and two comparison tests for cyclopentane at the standard pressure lower temperature and standard pressure and temperature as stated by ASTM D6890. It should be noted that the standard deviation at the normal test conditions are slightly higher than optimal when testing a standard diesel fuel, but is expected when testing a fuel with octane ratings above 90 (cyclopentane has an octane rating of approximately 94).

Table 1. Ignition Delay Results with Original Injector.

Pressure (bar)		1	1	21.4	21.4
Temp (K)		803	803	781	835
O ₂ (conc.)		13.3%	21%	21%	21%
IDT (ms)	Average	29	24.0	111.0	75.8
	Min	3.0	6.0	90.1	13.0
	Max	83.0	90.0	184.5	91.0
	Range	80.0	84.0	94.4	78.0
	Std Dev	24.0	23.9	21.4	13.2

Based upon these results, if cyclopentane comes in contact with stainless steel at these temperatures and pressures, it can ignite in the range of 3 to 90ms from the time of injection in 13.3% to 21% oxygen concentrations. It was postulated that this extremely small IDT could be the result of the extreme rich mixture and catalytic reactions from wall wetting. The IQT™ is constructed of stainless steel, a material that contains nickel. Nickel is known to catalytically decompose cyclopentane (Ginosar et al., 2011). It is apparent that the catalytic effects of the IQT materials of construction influenced the IDTs.

4.3 Experiments with Modified Injector

The large discrepancy in IDTs obtained from the tests conducted with combustion chamber pressures of 1 and 21.4 bar prompted a change in experimental setup. The standard nozzle was replaced by a Lucas BDN12SD12 (injector hole size of 1.011 mm) to reduce the amount of fuel injected and minimize wall wetting issues in the combustion chamber.¹¹ To correct the oxygen-to-fuel ratio for each run, the injector pump was removed, adjusted, and fitted with the new nozzle to allow for lower injected mass. The injection pump was recalibrated for the correct fuel mass at atmospheric pressure. The injector and pump assembly were calibrated by injecting 100 shots into a container, which were weighed to determine the mass per injection. This process was repeated until the desired fuel mass for stoichiometric combustion was achieved and then repeated three times to determine repeatability.

Two tests were performed with the modified injector. Both tests were performed using air with either a 13.3% or 21% O₂ concentration at 530°C and 1 bar. The results of these tests are shown in Table 2. The measured IDTs exhibit the trend of a longer ignition delay at the lower oxygen concentration. As the oxygen content is reduced from 21% (essentially atmospheric) to 13.3%, the IDT increases by more than a factor of two. The minimum measured IDT is 2.861 seconds for the conditions present in the ORC DE (i.e., 13.3% O₂ concentration, 803 K and 1 bar) system. Based upon these results, cyclopentane can ignite in the range of 2.8 to 3.8 seconds from the time of injection at 13.3% oxygen concentration and 1.4 to 1.8 seconds at 20.95% oxygen concentration at 1 bar pressure and 803 K.

Table 2. Ignition Delay Results with Modified Injector.

		O ₂ concentration	
		13.3%	21%
IDT (ms)	Average	3349	1568
	Min	2861	1355
	Max	3767	1801
	Range	906	446
	Std Dev	258	106

4.4 Experiments with Modified Injector for Vitiated Air at Different Equivalence Ratios

A third set of experiments were performed to investigate the IDT as a function of equivalence ratio and temperature. The initial experimental matrix consisted of equivalence ratios (Φ) from 0.5 to 3.0 and chamber temperatures ranging from 673 to 823 K. The equivalence ratio is defined as (Turns, 2006)

$$\Phi = \frac{\left(\frac{F}{A}\right)}{\left(\frac{F}{A}\right)_{stoic}}$$

where

$\left(\frac{F}{A}\right)$ is the fuel to air ratio of the mixture

$\left(\frac{F}{A}\right)_{stoic}$ is the stoichiometric fuel to air ratio

No ignition was detected for several of the test cases (for $\Phi = 0.5$ or $T \leq 773$ K), even though conditions were held for 15 seconds. A review of the test data concluded that the three cases not yet completed ($\Phi = 0.5$ and $T = 723$ K, $\Phi = 1$ and $T = 673$ K, and $\Phi = 1$ and $T = 723$ K) would have little propensity to ignite. The test matrix was modified to exclude those cases and extend the test conditions to include $\Phi = 5$ and $T = 773$ K, 803 K, and 823 K. Mixtures richer than $\Phi = 5$ were not investigated. Table 3 summarizes the revised test matrix and denotes whether or not ignition occurred. Table 4 shows the amount of fuel injected for each test case, along with the respective mass flow rates into the chamber. The approximate velocity of the flow through the nozzle is also listed.

Table 3. Test matrix.

Temperature (K)	$\Phi = 0.5$	$\Phi = 1$	$\Phi = 3$	$\Phi = 5$
673	No Ignition	<i>Not Tested</i>	No Ignition	<i>Not Tested</i>
723	<i>Not Tested</i>	<i>Not Tested</i>	No Ignition	<i>Not Tested</i>
773	No Ignition	No Ignition	No Ignition	IGNITION
803	No Ignition	IGNITION	IGNITION	IGNITION
823	No Ignition	IGNITION	IGNITION	IGNITION

Table 4. Fuel mass injected, mass flow rate and approximate velocity of flow from nozzle.

Temperature (K)	$\Phi = 0.5$	$\Phi = 1$	$\Phi = 3$	$\Phi = 5$
673	0.00238 g	0.00477 g	0.01430 g	–
	–	–	–	
723	0.00222 g	0.00443 g	0.01330 g	–
	–	–	–	
773	0.00208 g	0.00417 g	0.01250 g	0.02080 g
	–	–	–	27.8 g/s 46.1 m/s
803	0.00200 g	0.00400 g	0.01200 g	0.02002 g
	–	5.0 g/s 8.3 m/s	15.4 g/s 25.5 m/s	27.6 g/s 45.8 m/s
823	0.00195 g	0.00390 g	0.01170 g	0.01953 g
	–	6.3 g/s 10.4 m/s	15.1 g/s 25.0 m/s	28.7 g/s 47.6 m/s

Table 5 lists the average, minimum, maximum IDTs for the seven cases where ignition occurred. Of the cases tested, the average IDT ranges from 0.7 to 3.35 seconds, with a maximum and minimum IDT of 3.75 and 0.62 seconds respectively. The table also provides the range and standard deviation of the measurements. The range between the minimum and maximum observed IDTs can be as long as 1 second. It should be noted that the standard deviations are slightly higher than optimal when testing a standard diesel fuel, but are expected when testing a fuel with octane ratings above 90 (cyclopentane has an octane rating of approximately 94). However, for long ignition delay times, there might be sufficient time for some of the liquid fuel, if present, to settle onto the floor of the combustion chamber, increasing the standard deviation of the measurements.

Table 5. Measured ignition delay (ms) for vitiated air at atmospheric pressure.

IDT (ms)	$\Phi = 1$		$\Phi = 3$		$\Phi = 5$		
	803K	823K	803K	823K	773K	803K	823K
Average	3349.9	1358.9	1361.1	876.9	2302.1	1069.7	698.2
Min	2856.4	1040.0	1195.0	780.0	1860.0	975.0	620.0
Max	3751.8	1650.0	1483.0	1010.0	2885.0	1155.0	810.0
Range	895.4	610.0	288.0	230.0	1025.0	180.0	190.0
Std Dev	260.0	158.2	75.3	43.5	291.9	49.0	42.5

Since the exhaust gas cools from an inlet temperature of 803 K as it flows through the direct evaporator, a range of temperatures will be present. Also, a pinhole leak may produce air-to-fuel ratios other than stoichiometric to be present. The test matrix encompasses lean, stoichiometric, and rich conditions ranging from just above the autoignition temperature to slightly above the design TEG temperature. Such data are used to establish a set of ignition delay curves.

Figure 7 shows a plot of the logarithm of the average measured IDT for cyclopentane versus the inverse air temperature. The trend shows an increase in IDT as temperature decreases. The fuel-rich mixtures exhibit the smallest ignition delays. Similar trends are reported in the literature for cyclopentane and other fuels at higher pressures from lean to stoichiometric mixtures (Daley et al., 2008).

Figure 7. Average measured ignition delay time for cyclopentane.

4.5 Summary of Autoignition Experiments

In summary, and IQTTM apparatus was used to determine the IDTs for cyclopentane in vitiated air at atmospheric pressure. Further details of the IQTTM experiments in the sub-sections above have been published in the open literature (Guillen, 2012).

Due to the extremely low IDTs observed when cyclopentane comes into contact with stainless steel, it is imperative that stainless steel, or any material that behaves as a catalyst for combustion, be avoided as a material of construction for the ORCs with DEs designed to operate with cyclopentane as the working fluid and exhaust gas at temperatures above the autoignition temperature. For the tests run here, the observed IDT for cyclopentane injected into vitiated (13.3% oxygen) air is more than double that for atmospheric air (~21% oxygen).

IQTTM testing was performed for cyclopentane injected into vitiated air (13.3% oxygen) at equivalence ratios of 0.5, 1, 3, and 5 and chamber temperatures ranging from 673 to 823 K to establish a set of ignition delay curves. For these conditions, cyclopentane was observed to ignite in the range of 0.62 s ($\Phi = 5$, $T = 823$ K) to 3.75 s ($\Phi = 1$, $T = 803$ K) from the time of injection at 13.3% oxygen concentration and 1 bar pressure. The IDT was observed to decrease with increasing temperature and equivalence ratio. For the cases tested, no ignition was observed at temperatures at or below 723 K or at an equivalence ratio of 0.5. All of the cases tested at $\Phi = 5$ ignited.

Because of the nature of non-premixed combustion, the conditions tested by the current set of experiments may not have captured the minimum IDT for an ORC leak scenario. The fuel-rich mixtures exhibit the smallest ignition delays. Therefore, in a leak situation, it is expected that fuel-rich regions would ignite first.

5. COMPUTATIONAL FLUID DYNAMICS SIMULATIONS OF IQTTM CHAMBER

Computational fluid dynamics (CFD) was performed to investigate the mixing of cyclopentane with air, and resulting combustion, in an IQTTM chamber. A CFD model of the IQTTM chamber used in the experiments was created using STAR-CCM+ version 8.02.008. The approach taken here is to create a CFD model of the IQT to tune the combustion submodel using the autoignition data. The computational

procedure mimics the experimental tests. Initial conditions are prescribed within the computational domain and fuel is injected into the combustion chamber. Quiescent, vitiated air comprised of 13.3% O₂ and 86.7% N₂ at 803K fills the inside of the combustion chamber prior to injection. A fixed mass of cyclopentane was injected using a hollow cone injector with inner and outer angles of 5 and 15°. This narrow cone angle was used to represent the modified injector used in the experiments to avoid wetting the walls. Injection of cyclopentane into the computational domain is shown in Figure 8. Autoignition is detected by placing a pressure transducer within the domain. The pressure is monitored and a sharp rise in pressure signifies ignition.

Figure 8. Model of injection of cyclopentane into combustion chamber.

A Reynolds Averaged Navier Stokes (RANS) solver with a $k-\epsilon$ turbulence model was used. The mesh is constructed with a prism layer along the wall and polyhedral cells throughout the combustion chamber. The mesh contains a total of 2.5×10^5 polyhedral cells. The walls were prescribed as adiabatic with no-slip boundary conditions. Droplets that impact the walls evaporate. The specific heat was prescribed as a seven coefficient NASA polynomial function of temperature. Convection and time-differencing were set to second-order accuracy. A time step of 1.0×10^{-4} was necessary to achieve convergence.

Researchers at Ecole Nationale Supérieure des Industries Chimiques in France (Buda, 2005; Sirjean, 2007) have developed kinetic mechanisms for cyclopentane autoignition at temperatures from 1230 to 1800 K. However, a detailed chemical-kinetic mechanism for cyclopentane at the temperatures of interest for this application was not found in the literature. Therefore, DigAnaRS release DARS v2.08.002 was used to construct flamelet libraries for cyclopentane using a mechanism developed for n-heptane. The flamelet concept for non-premixed combustion describes the interaction of chemistry with turbulence in the limit of fast reactions (large Damköhler number). The combustion is assumed to occur in thin sheets with inner structure called flamelets. The turbulent flame itself is treated as an ensemble of laminar flamelets that are embedded into the flow field. Data on laminar flames are pre-calculated and stored in a library to reduce computational time. The main advantage of the flamelet model is that even though detailed information of molecular transport processes and elementary kinetic reactions are included, the numerical resolution of small length and time scales is not necessary. This avoids the well-known problems of solving highly nonlinear kinetics in fluctuating flow fields and makes the method very robust. Only two scalar equations are solved independent of the number of chemical species involved in the simulation.

A detailed reaction mechanism for n-heptane oxidation at 1 bar (Ahmed 2007) was used to create flamelet libraries at 773K, 803K and 823K. The flamelet library is then loaded into the CFD solver. Since cyclopentane is a product of n-heptane combustion, it was thought to be a reasonable choice, given that a

mechanism for cyclopentane combustion at the temperatures and pressures of interest was not available. The library generation tool can produce libraries using a reactor tool for a combustion model in either CFD or Engineering Science and Mechanics computations. The generation of flamelet libraries is very fast and robust and has been tested for various complex chemistry models. An ignition library can also be generated for different equivalence ratios for given fuel and air mixtures. This information can be used in a CFD computation to track ignition delays. This library generation tool provides the potential capability to combine turbulent interactions with complex chemistry for the turbulent reacting flow simulations.

Unfortunately, the ignition delays computed by the flamelet approach were orders of magnitude too small. An alternate approach was implemented to model the combustion. The combustion is modeled as a one-step reaction using the eddy-breakup (EBU) methodology. The EBU model assumes that the combustion rate is dominated by fluid mechanical rather than chemical phenomena. This is essentially a mixed-is-burned approach, wherein the chemical reaction rates play no role in determining burning rates; rather, combustion is completely controlled by turbulent mixing rates. Since turbulent mixing may be viewed as a cascade process from the integral down to the molecular scales, Spalding (1971) proposed that the cascade process also controls the chemical reactions as long as mixing rather than reaction is the rate determining process. Thus, the chemical time scale of an assumed one-step reaction is replaced by the turbulent time scale $\tau = k/\epsilon$ (where k is turbulent kinetic energy and ϵ is eddy dissipation). By doing this, the influence of chemical kinetics is eliminated, and the model represents the fast chemistry limit. When these models are used in CFD calculations, it turns out that the constants A and B must be “tuned” within a wide range in order to obtain reasonable results for a particular problem. The standard EBU model in STAR-CCM+ is used with the default coefficients, A equal to 4 and B equal to 0.5.

A mass of 0.005 kg/s of cyclopentane is injected over 8.0×10^{-4} seconds. The ignition delay is manually tuned to match the experimental data. The results from the eddy-breakup model were compared to the theoretically predicted adiabatic flame temperature (AFT) of the mixture. The computed maximum temperature is compared to the calculated AFT for cyclopentane in an environment comprised of 13.3% oxygen and 86.7% nitrogen. The corresponding ratio of oxygen to nitrogen is 1:6.52. A limiting flame temperature can be approximated by the AFT for a stoichiometric mixture of fuel and vitiated gases. The AFT is approximated by using average (rather than temperature-dependent) values for heat capacity. The calculation below assumes an initial temperature of 298 K the fuel and air. The reaction is described by the following equation:

The heat capacity of the products of reaction is given in Table 6.

Table 6. Heat capacity of reaction products (13.3% O₂/86.7% N₂).

	Thermal Capacity at 1000K		
	No. of Moles	J/Mol-K	J/K
CO ₂	5	54.3	271.5
H ₂ O	5	41.2	206.0
N ₂	48.9	32.7	1599.0
			2076.5

$$cp_{\text{sum}} := 2076.5 \cdot \frac{\text{J}}{\text{K}}$$

Heat of combustion, cyclopentane (NFPA 2002):

$$\Delta H_c := 3.098 \times 10^6 \text{ J}$$

$$\Delta T := \frac{\Delta H_c}{c_{p_{\text{sum}}}} = 1492 \text{ K}$$

$$T_{\text{ref}} := 298 \text{ K}$$

$$AFT := \Delta T + T_{\text{ref}} = 1790 \text{ K}$$

The AFT calculated in this ideal manner is the highest possible flame temperature for combustion in this air mixture. This calculated AFT is approximate and maximum because (NFPA 2002):

- Average values of c_p are used
- Heat losses due to radiation from hot gases (CO_2 and H_2O) are neglected
- Dissociation of products (carbon dioxide and water vapor) will occur at high temperature and these processes are endothermic.

Actual flames will be cooler than the AFT, since heat will be transferred from the flame to the surroundings by convection and radiation (Baukal and Schwartz 2001).

6. HEAT EXCHANGER MODEL

6.1 Methodology

To investigate flammability of the proposed direct evaporator design, a leak in the heat exchanger tubing was simulated using CFD. An analysis was performed for the evaporator section of the direct evaporator using STAR-CCM+ version 8.02.008 on a Dell Precision T5600 workstation with a 32 processor, Intel Xeon CPU E5-2687W @ 3.1 GHz processor running openSUSE 12.3. An initial computational mesh was created and preliminary runs made using a RANS- methodology. The RANS results were used to refine the mesh for a large-eddy simulation (LES). Although computationally intensive, an LES approach has the ability to more accurately represent details in the flow, especially where turbulent mixing and unsteady flow are present. LES is an inherently transient technique in which the large scales of the turbulence are solved for, and the small-scale motions are modeled. By modeling less of the turbulence and explicitly solving for more of it, the error in the turbulence modeling assumptions will not be as consequential. The smaller eddies are self-similar and will thus lend themselves to simpler, more broadly applicable models.

6.2 Governing Equations

The equations solved in the LES implementation are obtained by a filtering, rather than an averaging, process. The filtered equations may be rearranged into a form that looks virtually identical to unsteady RANS equations. For example, the filtered momentum equation is

$$\frac{\partial}{\partial t} \bar{\rho} \langle u_i \rangle + \frac{\partial}{\partial x_j} \langle u_i u_j \rangle = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

The filtered equations are discretized using the finite volume method in an unstructured, collocated grid arrangement with second-order accurate methods in space and time. Around 20 iterations are required for convergence of the equations within each time step to within a prescribed tolerance of 10^{-3} for the normalized residuals. The CFD simulation was run to convergence while the resolved kinetic energy was monitored with the goal of reaching a stationary kinetic energy. The model reached a stationary state in roughly 30 milliseconds of simulation time.

6.3 Geometry and Computational Mesh

The computational model consists of a staggered arrangement of spiral-wound, finned tubes with two or three rows of finned tubes across the width and six lengthwise. Nine whole and six half-tubes are included in the domain shown in Figure 10. Table 7 lists the pertinent design parameters of the finned tube design in the evaporator. The computational domain measures 0.608 m long by 0.151 m wide by 0.318 m high. The computational domain is described in a fixed Cartesian coordinate system (x, y, z). The x-axis lies along the streamwise (longitudinal) flow direction, the z-axis lies parallel to the cylinder axis (spanwise direction), while the y-axis lies perpendicular to both the x- and z-axis (transverse or cross-stream direction). An inlet development region of 0.0764 m (from inlet to center of the first tube) is specified. The outlet region was extended 0.178 m to avoid flow recirculation at the outlet and minimize the influence of the outlet boundary.

Figure 10. Section view of computational mesh.

Table 7. Tube bank description.

Design Parameter	Value
Tube outside diameter (mm)	39.37
Fin outside diameter (mm)	78.74
Effective diameter (mm)	48.82
Transverse pitch sT (mm)	118.11
Longitudinal pitch sL (mm)	102.36
Tube Wall Thickness (mm)	2
Fin Thickness (mm)	1.2
Fins spacing (mm)	5.08
Number of tube rows modeled	6
Fin Type	Solid
Tube inside-wall temperature (K)	506

The geometry was created as a computer aided design model in Unigraphics and exported as a Parasolid kernel. There were some skewed cells where the spiral fins intersect the tube, which necessitated importing the STL file into ProStar and performing a manual cleanup. A computational mesh with a total of 6.8×10^6 cells was generated in STAR-CCM+. A polyhedral mesh comprised of

176,108 cells is used for the solid domain. A hexahedron mesh comprised of 6,629,415 cells is used for the fluid domain. The computational grid is sufficiently fine near walls to produce a dimensionless wall distance (y^+) value of less than 1.0 at the first grid point away from the wall. There are no highly skewed grids, and grid distribution has been concentrated near the tube walls to provide a better description of the boundary layer. A substantial amount of grid points are also accommodated in the region between the cylinders to resolve the wake region.

For a LES, the criteria that the mesh must resolve the integral length scales was applied. Our procedure is to first conduct a RANS solution and then to set the cell size of the LES mesh so that the mesh resolves the integral length scale ($0.1643 k^{1.5}/\epsilon$, where k is turbulent kinetic energy and ϵ is eddy viscosity) throughout the entire domain. This was accomplished by the use of a custom field function in STAR-CCM+. Mesh sizing calculations for this analysis indicated that a mesh size of 1.0 mm is appropriate. A cross-section of the mesh is shown in Figure 11.

Figure 11. Section view of computational mesh.

6.4 Boundary Conditions, Properties, and Composition

The exhaust gas enters the inlet with the constant physical properties listed in Table 8 and the species composition listed in Table 9. In practice, a distribution grid upstream of the finned tube bank eliminates the swirl in the TEG and produces a uniform inlet profile to the tube bank. The flow velocity and temperature across the inlet boundary are assumed to be constant.

Table 8. Exhaust gas parameters.

Parameters	Value
Inlet velocity (m/s)	10.9
TEG mass flow rate (kg/s)	64
Duct area (m ²)	13.72
Inlet temperature (K)	803
Working fluid temperature (K)	506
Working fluid pressure (MPa)	4.176
Tube outside diameter (m)	0.0254
Fin outside diameter (m)	0.0508
Exhaust gas kinematic viscosity (m ² /s)	0.00008045

Table 9. Exhaust gas composition and mixture density (Incropera et al., 2007; Stewart and Jacobsen, 1989).

Constituent	Mole Fraction, Y_i	Density, ρ_i (kg/m ³)
N ₂	0.7476	0.4211
O ₂	0.1331	0.481
H ₂ O	0.076	0.2739
CO ₂	0.0344	0.6614
Ar	0.0089	0.6084
Mixture	1	0.4278

The Synthetic Eddy Method in STAR-CCM+ is implemented to generate turbulent eddies across the inflow boundary to provide an initially perturbed flow field. A constant pressure boundary is set at the downstream end of the computational domain. No-slip conditions are imposed on solid surfaces (tubes and fins). Periodic boundary conditions are applied on the top, bottom, and sides of the domain. An isothermal condition is imposed on the tube inner walls, set equal to the average temperature of working fluid circulating inside the tubes. A uniform inside-wall temperature of 506 K is specified for the tubes. The conjugate method allows for a coupled heat transfer solution between the solid and fluid. This involves creating an in-place interface between the wall boundaries enclosing each of the two regions, and then defining this interface as being an appropriate contact type for fluid-solid heat transfer. A contact-type interface between the fluid and solid regions is implemented. The condition imposed at the solid-fluid interface to conserve heat flux across the boundary can be expressed as

$$T_{\text{solid}} = T_{\text{fluid}}, \text{ or } -k_s \frac{\partial T_s}{\partial n} = -k_f \frac{\partial T_f}{\partial n}$$

where

T = temperature (K)

k = thermal conductivity (W/m-K)

n = direction normal to interface.

The tube material SA192 or SA110A1 for the pipes (carbon steel) and fin material is A366 (mild carbon steel). All fins are helically wound, solid fins.

6.5 Supporting Calculations

The calculation of AFT based upon the TEG mixture given in Table 9 above is as follows:

The heat capacities of the products of reaction are given in Table 10.

Table 10. Heat capacities of the products of reaction (actual TEG mixture).

	Thermal Capacity at 1000K		
	No. of Moles	J/Mol-K	J/K
CO ₂	6.94	54.3	376.8
H ₂ O	9.28	41.2	382.3
N ₂	42.1	32.7	1376.7
Ar	0.5	20.8	10.4
			2146.2

$$cp_{\text{sum}} := 2146.2 \cdot \frac{\text{J}}{\text{K}}$$

Heat of combustion in TEG calculated using heats of formation (NFPA 2002):

$$\Delta H_c := 6.94 \cdot (-393.5 \cdot 10^3 \text{ J}) + 9.28 \cdot (-241.8 \cdot 10^3 \text{ J}) - (-77.45 \cdot 10^3 \text{ J}) = -4.897 \times 10^6 \text{ J}$$

$$\Delta T := \frac{-\Delta H_c}{cp_{\text{sum}}} = 2282 \text{ K}$$

$$T_{\text{ref}} := 298 \cdot \text{K}$$

$$AFT := \Delta T + T_{\text{ref}} = 2580 \text{ K}$$

The Reynolds number was calculated based upon an effective diameter, D_e , for the finned tubes. The value of the effective diameter was calculated based on the formula given by Mair et al. (1975)

The value of the effective diameter was calculated based on the formula given by Mair et al. (1975)

$$D_e = \frac{(s - t)D + tD_f}{s}$$

where

s = fin spacing

t = fin thickness

D = tube outer diameter

D_f = outer fin diameter

as illustrated in Figure 12. From the above formula, the effective diameter for the specified finned tubing is 0.0314 m. The effective diameter accounts for the increase in flow blockage caused by the fins.

Figure 12. Parameters used in calculation of effective tube diameter (Ziada et al., 2007).

6.6 Leak Scenario

The leak scenario consisted of a simulated pinhole leak in thin wall tubing. The leak was modeled as injection from a volumetric source located at either the 9, 6, or 3 o'clock positions on the tube. The mass flow rate emanating from the leak corresponded to a 25.4 micron pinhole in the middle tube of the third row. Since the boiling point of cyclopentane at atmospheric pressure is <322.4 K, the leaked fluid flashes to vapor nearly instantly. Mass flux is driven by concentration gradients via the off-diagonal terms in the conservation equations. Mixing across streamlines occurs due to diffusion. It is important to note that tracer particles could not simply be injected at the inlet to simulate a pinhole leak. The particles would simply follow the streamlines and be whisked downstream in a fraction of a second. By injecting the particles at various circumferential positions on the tube, the particles have the opportunity to be caught up in the wake region behind the tube. If the particles released into the hot TEG were simply to follow streamlines and do not get caught up in the tube wake, it can be shown that the residence time of the released particles at the inlet is several orders of magnitude lower than the minimum measured IDT in the experiments.

For instance, a flaming soot particle entrained in the TEG flow entering the inlet of the heat exchanger would be whisked downstream through the exit in a fraction of a second. Since the particle would typically follow a streamline, it would exit the heat exchanger before it had sufficient time to cause structural damage to the finned tubes. The overall length of the heat exchanger, including evaporator, superheater and economizer, is 2.22 m. At a TEG flow velocity of 10.9 m/s, the time for a particle to traverse the length of the heat exchanger is 0.2 s (200 ms).

A Lagrangian formulation with tracer particles injected was invoked to visualize the leaked fluid flow and transport through the heat exchanger. Residence time of the particles provides information as to how long the leaked fluid would remain in the heat exchanger. Cyclopentane was injected at the rear of the tube (the 3 o'clock) position, since a leak at this location was found to be the worst case from the standpoint of fluid hold up in the wake. Particle trajectories were calculated using the Lagrangian method.

Leak rates were calculated assuming choked flow through an orifice. If the working fluid is released from a supply pressure of 44 bar to atmospheric pressure through a pinhole the size of 0.001 inches (127 μm), the resulting leak rate is 5.818×10^{-6} kg/s. Three leak locations were simulated at the: rear of tube (3 o'clock position), side of tube (6 o'clock position), and front of tube (9 o'clock position). Release rates are calculated in the Appendix for various pinhole leak sizes.

6.7 Results and Discussion

The fluid domain was initialized with a uniform velocity equal to the inlet velocity specified in Table 7. The TEG flow accelerates through the gaps between the tubes, as seen by the higher velocities in Figure 13. Stagnant flow in the recirculation regions behind the tubes is clearly seen in the cut through the x-y mid-plane. The flow exhibits the expected vortex shedding behavior for flow over a staggered tube bank. Higher flow velocity is seen between the fins in the cut through the y-z mid-plane.

(a)

(b)

Figure 13. Instantaneous velocity magnitude distribution: (a) cut through x-y mid-plane, (b) cut through y-z mid-plane.

Recirculating flow in the wake regions can be clearly seen in the snapshot of velocity vectors in Figure 14. Regions of slower velocity and recirculation behind the tubes are evident. The literature shows that the flow and heat transfer from the tube bundle is affected by the arrangement of tubes (Buyruk, 1999). The flow accelerates as it passes through the narrower region between the tubes. Flow past the tubes is affected by flow acceleration and blockage from the upstream tubes. Flow at the rear of the tubes is affected by the turbulence from the adjacent tubes.

Figure 14. Instantaneous velocity vectors.

Figure 15 shows a close-up view of the streamlines near the intact tubes. As flow velocity at the rearward side of the tube decreases, the pressure increases and the energy in the flow is insufficient to overcome the increasing pressure, thus separating the flow from the surface. Energy is consumed in overcoming the boundary layer friction. Separation of the boundary layer takes place when low velocity fluid adjacent to the tube wall cannot overcome the adverse pressure gradient at the rear portion of the tube and the flow reverses direction. The boundary layer separates from the tube at an angle of approximately 100 degrees. Fluid movement starts to curl and gives rise to vortices the shed from the tube.

The recirculation region in the wake is the distance from the rear stagnation point of tubes to the end of recirculation bubble where the time-averaged streamwise velocity along the centerline in the wake changes from the negative or positive values to a zero value. Balabani (1996) performed measurements downstream of the third cylinder at a gap Reynolds number, Re_{gap} , varying from 3,104 to 12,858 and provided the following correlation for the length of the recirculation zone, l_r .

$$\frac{l_r}{D} = -0.69 \log(Re_{gap}) + 3.8$$

The length of the recirculation zone was measured from the center of the corresponding cylinder. Results from the correlation, using the effective diameter for D , are in good agreement with the CFD results. The correlation predicts that the recirculation length is slightly greater than the effective diameter of the finned tubes. The length of the recirculation region is roughly 0.04 m long or 1.1 times the effective tube diameter. Figure 16 shows the distribution of Reynolds number in the exhaust gas flow. The effective tube diameter calculated in Section 6.5 was used to calculate Reynolds number.

Figure 15. Flow separation from tube.

Figure 16. Reynolds number of exhaust gas flow.

The temperature distribution was determined by solving the conjugate heat transfer problem for the fluid and solid computational domains. Figure 17 shows a screenshot of a cut-plane through the heat exchanger with the temperature distribution prior to combustion of the leaked working fluid. The finned tubes are effective at transferring heat from the TEG to the working fluid, as seen by the decreasing temperature as the TEG proceeds toward the outlet. In this figure, streamlines are overlaid on contours of constant temperature. When the isotherms are perpendicular to the local streamlines, there is excellent synergy between the velocity field and the temperature field (Chen et al., 2010). Conversely, when the isotherms are parallel to the local streamlines, it indicates a poor synergy between the velocity field and the temperature field (Chu et al., 2009). Consequently, the wake is the poorest heat transfer region, which is beneficial from an autoignition standpoint. The wake region is noticeably cooler than the other regions in the flow domain. Prior to combustion due to a pinhole leak, TEG in the wake region is below the autoignition temperature for cyclopentane.

Figure 17. Streamlines overlaid on temperature contours for conditions prior to leak.

The primary concern in this study is the potential for leaked working fluid to become trapped in the recirculation regions aft of the finned tubes and autoignite. The stabilization of a flame in the eddy region behind a bluff body in a high velocity gas stream is a well-known phenomenon used to anchor the flame in the combustors of jet engines (Longwell et al., 1953). A flame stabilized in this manner can spread throughout the entire flammable mixture. The residence time of gases in the recirculation zone behind a bluff body dictate whether the flame will propagate or extinguish. The scenario of concern is that fluid released through a small leak in a finned tube could ignite, burn undetected for a long time, and potentially degrade surrounding materials or ignite secondary fires.

From the ignition delay time published in the literature, it is evident that the container wall has an influence on the hydrocarbon oxidation. Mastorakos et al. (1997) attributes the likelihood of vortex cores igniting first to the fact that the concentration and temperature are fairly uniform at the center of the vortex, implying that there is little to no heat loss. The relatively large heat losses caused by turbulence in the other regions of the flow field tend to increase the autoignition delay time, since the rate of heat production by the chemical reaction is slower than the rate of heat loss. When heat losses at the system boundaries are completely balanced by heat generation resulting from the exothermal chemical reactions, such steady-state thermochemical conditions do not result in autoignition (Kolaitis and Founti, 2009).

The flow is expected to exhibit unsteadiness because of vortex shedding from the cylindrical tubes and the turbulent fluctuations (Johnson, 2008). Turbulent flow is characterized by fluctuations over a large range of scales. Fluctuations at different scales interact with each other and exchange momentum and energy. Turbulent transport can be regarded as diffusive in nature. As a result of mixing between turbulent eddies of all sizes, turbulent transport is a much more effective process than molecular transport, which is a very slow process on a macroscopic scale. Experiments for finned tubes in cross-flow performed by Ziada et al. (2005) show that the presence of fins on the tubes enhances vortex shedding.

A simulation was performed wherein the cyclopentane is released from the tube as a continuous spray. Combustion was modeled using the same EBU model as was used for the IQT™ simulations. A worst case scenario was run, wherein the leaked fuel is burned as soon as it is released into the TEG. Figure 18 shows the mass fraction of cyclopentane emanating from a pinhole leak located at the 3 o'clock position on the heat exchanger tube. Similar calculations were performed for cyclopentane leak positions at the leading edge (9 o'clock) and the bottom (6 o'clock) positions on the tube. These simulations (not shown) indicate that release from other positions is carried downstream and rapidly diluted with little residence time near the tube, so while a leak in other positions might pose a risk of a stable flame there appears to be far more risk of a stable flame if the leak is caught up in the wake of the tube. Attention was

thus focused on the case of a leak at the 3 o'clock position. Mass injected at the stagnation region of the tube is the most favorable aerodynamic condition for flame stabilization. Fuel in the regions away from the stagnation regions have less favorable aerodynamic conditions due to the higher flow velocities and shear. Figure 19 shows the flame resulting from a mixed-is-burned scenario (e.g., zero IDT). The tracer particles used to compute residence time were enlarged for visualization purposes. From the transient simulation of the particle transport over a 3 s injection time, the maximum residence time of a particle in the wake is 1.222 s. This occurs for a single particle that is caught up in the wake behind the tube with the leak. However, the median particle residence time is around 0.3 s. The residence time in the wake at the 3 o'clock position seems far too short for autoignition to occur when compared to the IDT obtained from the experiments.

Figure 18. Mass fraction of cyclopentane released.

Figure 19. Cut-plane image during combustion with particle residence time overlaid on isocontours of temperature.

Figure 19 shows isocontours of temperature within the heat exchanger due to combustion of the leaked cyclopentane into the hot TEG. The simulation shows the transport of tracer particles, colored by residence time. The computed maximum temperature of the flame is 1821 K. The diffusion flame is transported through the heat exchanger and its main effect is on the finned tube immediately downstream

of the leak. The computed maximum temperature in the finned tubes (1234 K) occurs on the fins of the middle tube in the fifth row (Figure 20). In this scenario, the fins are kept relatively cool by the 506 K cyclopentane inside of the tubes, which serve as a heat sink. Depending upon the type of carbon steel used in the construction, the melting temperature ranges from 1628 to 1813 K (Perry and Green, 2007). Therefore, the finned tubes would not be expected to melt.

Figure 20. Temperature distribution of solid fins resulting from combustion.

7. SUMMARY AND CONCLUSIONS

In summary, experiments at atmospheric pressure were conducted to obtain the IDT for cyclopentane in vitiated air (13.3% O_2) as a function of temperature and equivalence ratio. The experiments encompassed temperatures from 673K to 830K and equivalence ratios from 0.5 to 5. No ignition was detected for equivalence ratios of 0.5 and temperatures below 773 K. Of the cases where ignition occurred, the longest and shortest average IDTs were 3.35 s ($\Phi = 1$, $T = 803$ K) and 0.7 s ($\Phi = 5$, $T = 823$ K).

A CFD simulation was performed for the IQT chamber to obtain the appropriate parameters for the heat exchanger simulation. The combustion was calibrated to match the experimental data obtained using the IQT chamber. Then, a three-dimensional, transient CFD simulation of the evaporator section of the Direct Evaporator was performed using an LES methodology. Hot TEG flowing across a heat exchanger tube bank section interacting with ORC working fluid released from a pinhole leak at various locations from a tube was examined. The wake region was determined to be the area of most concern. Particles not caught up in the wake would simply be carried downstream along streamlines before they had the chance to autoignite. The CFD model was created to determine the residence time of leaked fluid held up in the wake and the temperature of the fluid in the wake.

At the flow conditions investigated, fluid released from a pinhole leak at 6 and 9 o'clock positions on the tube would not be caught up in the wake, but rather swept downstream before autoignition could occur. Fluid released from the 3 o'clock position on the tube enters the wake, but does not remain there

for a long enough period of time to initiate combustion. This makes the possibility of a fire in the heat exchanger unlikely.

Worst case simulations were performed to estimate the fluid and finned tube temperatures if combustion were initiated as a result of a leak. The simulation shows that the finned tubes would not reach their melting temperature from exposure to the diffusion flame.

8. RECOMMENDATIONS

To minimize the potential for a deflagration, a defense-in-depth strategy is recommended. The following precautions are advised:

- Specify seamless tubes to avoid the possibility of weld seam defects.
- Avoid contact of cyclopentane with stainless steel or other material that could catalyze combustion reactions.
- Purge the oxygen from the system with an inert gas (such as nitrogen) before system startup.
- Do not allow flammable/explosive concentrations of cyclopentane-TEG mixtures to stagnate. Maintain a minimum TEG flow through the heat exchanger. It is advisable to sweep such mixtures through the system to the flare.
- Incorporate hydrocarbon sensors to detect leaks. If a leak is detected, divert hot gas to the bypass stack, depressurize the cyclopentane system and flush with an inert gas.
- Exclude ignition sources whose energy is greater than the minimum ignition energy for the flammable mixture and enclose any ignition sources in an explosion-proof enclosure, which will not allow propagation of the flame out of the enclosure.
- Implement a nitrogen purge to extinguish any flames, as described in the following patents:
 1. Fire Extinguishing System for an Organic Rankine Cycle Hydrocarbon Evaporator, US20120023943A1, Feb. 2, 2012 – This invention provides an ORC energy recovery system comprising features which provide for fire suppression and/or ignition suppression in the event of an unintentional release of a flammable component of the system, for example a flammable working fluid such as cyclopentane, into a part of the system in which the prevailing temperature is higher than the autoignition temperature of the flammable components. In one embodiment, the ORC energy recovery system comprises an inert gas source disposed upstream of a hydrocarbon evaporator and is configured to purge the hydrocarbon evaporator with an inert gas on detection of a leak.
 2. Inert Gas Purging System for an ORC Heat Recovery Boiler, US 20120000200A1, Jan. 5, 2012 – System includes a valve system switchable between a waste heat recovery position configured to direct incoming exhaust gas through an interior volume of an exhaust section of an engine and a bypass position configured to direct the incoming exhaust gas through a bypass duct to bypass a heat recovery boilers within the interior volume. The system also includes an inert gas purging system configured to inject an inert gas into the interior volume to displace residual exhaust gas from the interior volume.

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Appendix A

MASS FLOW RATE FROM LEAK

Calculation of release rate of working fluid from heat exchanger tube for various leak sizes:

Choked flow through orifice

$$\rho := 170.6 \cdot \frac{\text{kg}}{\text{m}^3} \quad \text{Density of vapor}$$

$$P := 4.4(10)^6 \cdot \text{Pa}$$

$$k := 1.1217$$

$$D_{\text{tube}} := 1 \cdot \text{in}$$

Pinhole size:

$$i := 0..3$$

$$D_o := \begin{pmatrix} 0.005 \\ 0.001 \\ 0.0005 \\ 0.0001 \end{pmatrix} \cdot \text{in}$$

$$D_o = \begin{pmatrix} 0.127 \\ 0.0254 \\ 0.0127 \\ 0.00254 \end{pmatrix} \cdot \text{mm}$$

$$D_o = \begin{pmatrix} 127 \\ 25.4 \\ 12.7 \\ 2.54 \end{pmatrix} \cdot \mu\text{m}$$

$$\beta := \frac{D_o}{D_{\text{tube}}}$$

$$\beta = \begin{pmatrix} 5 \times 10^{-3} \\ 1 \times 10^{-3} \\ 5 \times 10^{-4} \\ 1 \times 10^{-4} \end{pmatrix}$$

$$Re_v := 2.034 \cdot (10)^6$$

$$C := 0.7092 \cdot \beta^2 - 0.4397 \cdot \beta + 0.6626$$

Regressed from Crane p. A-20

Release rate from pinhole:

$$\dot{m}_{o_i} := C_i \cdot \frac{\pi}{4} \cdot (D_{o_i})^2 \cdot \sqrt{k \cdot \rho \cdot P \cdot \left(\frac{2}{k+1} \right)^{\frac{(k+1)}{(k-1)}}}$$

$$\dot{m} = \begin{pmatrix} 1.451 \times 10^{-4} \\ 5.818 \times 10^{-6} \\ 1.455 \times 10^{-6} \\ 5.821 \times 10^{-8} \end{pmatrix} \frac{\text{kg}}{\text{s}}$$

$$P_2 := 1.4895 \cdot (10)^6 \text{ Pa}$$

$$\frac{P}{P_2} = 2.954$$

$$\left(\frac{k+1}{2} \right)^{\frac{k}{k-1}} = 1.724$$

since $P/P_2 > 1.724$, flow is choked

$$\dot{m} = \begin{pmatrix} 1.451 \times 10^{-1} \\ 5.818 \times 10^{-3} \\ 1.455 \times 10^{-3} \\ 5.821 \times 10^{-5} \end{pmatrix} \cdot \frac{\text{gm}}{\text{s}}$$