FINITE ELEMENT MODEL OF A HEATED WIRE CATALYST IN CROSS FLOW

Final Report
KLK752
Compression Ratio and Catalyst Aging Effects on Aqueous Ethanol
N09-03

National Institute for Advanced Transportation Technology
University of Idaho

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April 2009
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1. **Report No.**

2. **Government Accession No.**

3. **Recipient’s Catalog No.**

4. **Title and Subtitle**

   Compression Ratio and Catalyst Aging Effects on Aqueous Ethanol: Finite Element Model of a Heated Wire Catalyst in Cross Flow

5. **Report Date**

   April 2009

6. **Performing Organization Code**

   KLK752

7. **Author(s)**

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8. **Performing Organization Report No.**

   N09-03

9. **Performing Organization Name and Address**

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   PO Box 440901; 115 Engineering Physics Building
   Moscow, ID 838440901

10. **Work Unit No. (TRAIS)**

11. **Contract or Grant No.**

    DTRT07-G-0056

12. **Sponsoring Agency Name and Address**

    US Department of Transportation
    Research and Special Programs Administration
    400 7th Street SW
    Washington, DC 20509-0001

13. **Type of Report and Period Covered**


14. **Sponsoring Agency Code**

    USDOT/RSPA(DIR-1)

15. **Supplementary Notes:**

16. **Abstract**

   Our project seeks to advance catalytic plasma torch (CPT) technology through reactor studies, engine design, modeling, and engine testing activities. This report discusses our efforts to ignite lean homogeneous air-fuel mixtures in engines under conditions approaching Homogeneous Charge Compression Ignition (HCCI). An evaporator for low-density liquids including ethanol and water was developed, tested, and installed. Our initial experiments were conducted to measure the temperature of a heated platinum wire exposed to propane, oxygen, and water vapor for development of a one-step model of catalytic ignition of propane and oxygen on platinum. In the future, we intend to enclose the reactor to measure the conversion efficiency of fuel to combustion products. These experiments will require a water cooled nitrogen quenching probe, which was designed and built. Experimentally obtained temperatures of a heated coiled platinum wire in low Reynolds Number cross-flow were compared with a three-dimensional finite volume model. The calculated average wire temperature was in good agreement with experimentally obtained values with deviations close to experimental uncertainty bounds at temperatures between 530K and 815K. The rate of heat generated at the wire surface from catalytic reactions was found for the ignition of lean propane/oxygen/nitrogen mixtures.

17. **Key Words**

   Pollutant control, fuel systems, engine testing, renewable fuels

18. **Distribution Statement**

   Unrestricted; Document is available to the public through the National Technical Information Service; Springfield, VT.

19. **Security Classif. (of this report)**

   Unclassified

20. **Security Classif. (of this page)**

   Unclassified

21. **No. of Pages**

   21

22. **Price**

   …

Form DOT F 1700.7 (8-72)  Reproduction of completed page authorized
TABLE OF CONTENTS

1. Introduction .................................................................................................................................................. 1
2. Background ..................................................................................................................................................... 2
3. Methods .......................................................................................................................................................... 4
   3.1 Governing Equations .............................................................................................................................. 4
   3.2 Drawing and Meshing ............................................................................................................................. 4
   3.3 Preprocessing and Solver Parameters .................................................................................................. 7
4. Results ............................................................................................................................................................ 12
5. Summary and Conclusions ....................................................................................................................... 17
6. Acknowledgements ..................................................................................................................................... 18
7. Nomenclature ............................................................................................................................................... 19
8. References .................................................................................................................................................... 20

LIST OF FIGURES

FIGURE 1: Experimental set-up.......................................................................................................................... 2
FIGURE 2: Procedure for calculating surface reaction rate heat generation ................................................... 3
FIGURE 3: Platinum coil in quartz tube ............................................................................................................ 6
FIGURE 4: Preliminary gambit mesh; 237,107 elements. ............................................................................... 6
FIGURE 5: Gambit detailed mesh, 312,189 elements ..................................................................................... 7
FIGURE 6: FLUENT velocity contours in the flow around the coil and heated wire. ................................. 11
FIGURE 7: Measured velocity profiles near the coil ...................................................................................... 11
FIGURE 8: Coiled wire and flow temperature contours with power set to 9 W. ...................................... 12
FIGURE 9: Temperature distribution of the coiled wire with power set to 9W ........................................ 13
FIGURE 10: Average wire temperature vs. power plot ............................................................................... 14
FIGURE 11: Temperature vs. power plot including experimental uncertainty ......................................... 16

LIST OF TABLES

TABLE 1: Summary of Material Property Settings ....................................................................................... 8
TABLE 2: Summary of Boundary Condition Settings .................................................................................... 9
TABLE 3: Summary of Model Settings .......................................................................................................... 10
TABLE 4: Average Temperatures ................................................................................................................ 14

Finite Element Model of A Heated Wire Catalyst in Cross Flow
1. INTRODUCTION

A finite element modeling program was used to determine the average temperature of a platinum wire catalyst with internal energy generation subjected to a cross-flow. The results were compared to experimental data found by heating the platinum wire catalyst with a constant electric current. This information will be used in the further development of catalytic igniter technology for use in lean burning internal combustion engines [1-3]. It will aid in determining the average heat flux from a platinum surface and the power input necessary for the igniter to initiate combustion.

Our research team has a long-term interest in aiding the development of catalytic igniters for combustion of very lean mixtures in internal combustion engines. Prior work focused on the combustion of ethanol/water/air mixtures in different engine platforms [4, 5], a demonstration vehicle fueled with ethanol-water blends [6], and ignition of heavy fuels in small, low compression-ratio engines [7]. Catalytic ignition of homogeneous charges of aqueous fuels in high compression ratio engines promises improved efficiency and lowered emissions, especially NOx and particulates [8].

The work presented here represents progress towards our goal of studying the detailed behavior of catalysts exposed to ethanol/water/oxygen/nitrogen blends. To gain confidence in our experimental apparatus and methods, we started with dry propane/oxygen/nitrogen blends.
2. BACKGROUND

A plug-flow reactor was used to determine ignition temperatures of non-flammable propane/oxygen/nitrogen mixtures over a coiled platinum wire catalyst. The experimental schematic is shown in FIGURE 1 [9].

The platinum catalyst was electrically heated with an HP6673A variable power supply, operated in constant current mode. Data was collected for fixed volume percentages of oxygen, from 5 percent $\leq x_{O_2} \leq$ 20 percent in 2.5 percent increments and for fixed volume percentages of propane, from 1 percent $\leq x_{C_3H_8} \leq$ 2 percent in 0.5 percent increments. All experiments were run through an equivalence ratio, $\varphi$, from 0.1 $\leq \varphi \leq$ 1 in 0.2 increments, all while maintaining a non-flammable mixture at a total volumetric flow rate of 5 L/min. For these experiments, $\varphi$ is
defined as the ratio of the mass of propane to oxygen divided by an equivalent stoichiometric ratio. At each equivalence ratio, an HP3486A multi-meter was used to measure the voltage drop across the wire, from which the resistance and the average wire temperature were determined. These temperatures were plotted with respect to the power input to the wire and then compared to the average temperature with just air flowing over the coil. With this comparison the heat generation due to surface reactions could be calculated by the process shown in FIGURE 2. Point 1 marks the power input value where surface reactions begin to occur and increase the temperature up to Point 2. The power required to maintain this new temperature in air is marked by Point 3, so the difference in power between Points 1 and 3 is the heat generated from catalytic surface reactions. Hence, the measurement of the average wire temperature also provides the rate of heat generation, which is useful for catalytic igniter development.

The current FLUENT software model calculates the temperature of a heated coil exposed to a cross-flow of air.

**FIGURE 2: Procedure for calculating surface reaction rate heat generation.**
3. METHODS

3.1 Governing Equations

For the modeling, we used the Navier-Stokes momentum equations, Eq.1-3, along with the energy balance, Eq. 4, as the governing equations. The boundary conditions for these equations can be described with the FLUENT settings. We set the model to inviscid flow to create the plug-flow within the quartz tube. This gives a shear stress equal to zero at the quartz tube walls. However, the shear stress was accounted for along the coil walls; the velocity at the coil surface equals zero. An energy balance is performed at the interface of the fluid and the coil wall. At this point, the energy generated within the coil has to equal the energy transferred to the surroundings by conduction, convection, and radiation. The temperature boundary conditions used included setting the ends of the wire at a fixed temperature, and then due to symmetry, the change in temperature with respect to x along the coil length would be zero at the midpoint. Lastly, the temperature of the fluid was assumed to approach free-stream temperature at the edge of the thermal boundary layer around the coil.

\[
\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + \frac{u_g u}{r} \frac{\partial u}{\partial \theta} + u_z \frac{\partial u}{\partial z} + u_{r g} \right) = -\frac{\partial p}{\partial r} + \mu \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{2}{r^2} \frac{\partial u}{\partial \theta} - \frac{u_r}{r^2} \right] + \rho g_r 
\]

(1)

\[
\rho \left( \frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial r} + \frac{u_g \phi}{r} \frac{\partial \phi}{\partial \theta} + u_z \frac{\partial \phi}{\partial z} + u_{r g} \right) = -\frac{\partial \phi}{\partial r} + \mu \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{2}{r^2} \frac{\partial \phi}{\partial \theta} - \frac{u_r}{r^2} \right] + \rho g \phi 
\]

(2)

\[
\rho \frac{DU}{Dt} = \nabla \cdot \left( k \nabla T \right) + \frac{Dp}{Dt} + \Phi 
\]

(3)

(4)

3.2 Drawing and Meshing

Two models were run using FLUENT: 1) a preliminary model and 2) a more detailed model with more accurate radiation parameters. The preliminary model included the wire and air only, with the wire modeled as a blackbody. The more detailed modeled also included the quartz tube, but the change that affected the model most was including the emissivity of platinum which is dependent on temperature. For each model, a SolidWorks™ drawing of the coil and quartz tube

Finite Element Model of A Heated Wire Catalyst in Cross Flow
configuration was made. The first included a 127 micron diameter coil having a total length of approximately 13.208 cm. The air volume around the coil was also included, with a diameter of 2.7305 cm, the inside diameter of the quartz tube. The second drawing was similar, but included the quartz tube with a 3.29 cm outside diameter, as well as, longer wire ends to represent the entire 14.224 cm of coil between the lead clips. Once these drawings were complete, they were imported into Gambit to be meshed. The meshes were created by first meshing the edges, then surfaces, and finally the volumes. This was to ensure there was a fine enough grid at the critical points around the wire to produce accurate results. Figure 3 shows the coil in the quartz tube; the intensity of the glowing wire overwhelms the camera. The meshed drawings can be seen in Figures 4 and 5.
FIGURE 3: Platinum coil in quartz tube.

FIGURE 4: Preliminary gambit mesh; 237,107 elements.
3.3 Preprocessing and Solver Parameters

Next, the materials and boundary conditions were defined in FLUENT. For the preliminary model, platinum had to be added to the database by inputting values for density, specific heat, and thermal conductivity. Air was already defined as a material; however, it was found that the results became much closer to those found experimentally once the specific heat and thermal conductivity of air were input as functions of temperature. For the more detailed model, radiation properties had to be input for each material. These properties included absorption coefficient, scattering coefficient, scattering phase function, and refractive index. For all three materials platinum, quartz, and air, the scattering phase function was left as isotropic, the default selection. For platinum, an opaque solid, and air, a non-participating media, the absorption and scattering coefficients can be assumed to equal zero. Quartz is semi-transparent but spectral variation in ability to absorb cannot be specified in FLUENT. Therefore, the model was run with the properties of quartz set at the extremes of being either transparent or opaque; the results only differed by 0.01 K. Lastly, the index of refraction, n, was entered for each of the materials as 2.33, 1.46, and 1 for platinum, quartz, and air respectively. The material property inputs for air, platinum, and quartz are summarized in Table1.
TABLE 1: Summary of Material Property Settings

<table>
<thead>
<tr>
<th>Property</th>
<th>Air</th>
<th>Platinum</th>
<th>Quartz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m$^3$)</td>
<td>1.225</td>
<td>21,450</td>
<td>2,620</td>
</tr>
<tr>
<td>Specific Heat (J/kg-K)</td>
<td>1050-0.365<em>T+8.5E-04</em>T$^2$-3.7E-07*T$^3$</td>
<td>130</td>
<td>830</td>
</tr>
<tr>
<td>Thermal Conductivity (W/m-K)</td>
<td>-3.93E-04+1.02E-04<em>T-4.86E-08</em>T$^2$+1.52E-11*T$^3$</td>
<td>71.6</td>
<td>1.46</td>
</tr>
<tr>
<td>Viscosity (kg/m-s)</td>
<td>1.789E-05</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Absorption Coefficient (1/m)</td>
<td>--</td>
<td>1</td>
<td>4.5</td>
</tr>
<tr>
<td>Index of refraction</td>
<td>1</td>
<td>2.33</td>
<td>1.46</td>
</tr>
</tbody>
</table>

Boundary conditions were set for each of the faces as well as all volumes (see Table 2). The velocity of the air was set on the inlet face, with a value of 0.173 m/s and a temperature of 290K with the outlet set as outflow. The coil wall face was given a no slip boundary condition, as well as an emissivity. This emissivity varies with temperature, so it is chosen using the average wire temperature expected from the experimental results. A curve was calculated using emissivity data from a literature search [10-16]. The resulting piece-wise function is shown in Eq. 5 and 6.

Platinum emissivity as a function of temperature:

For $T < 582$ K:
\[
\varepsilon = 1.65 \times 10^{-4} T - 1.6378 \times 10^{-2}
\]  
(5)

For $T > 582$ K:
\[
\varepsilon = -5.23 \times 10^{-8} T^2 + 2.34 \times 10^{-4} T - 3.84 \times 10^{-2}
\]  
(6)

All remaining faces were set as walls with zero shear stress on the air flow. The quartz tube faces were each given an emissivity of 0.93. The ends of the wire were fixed to remain at 290K, due to the thermal inertia from the relatively large metal clips on the power supply leads. Each volume was set to participate in radiation, and finally the coil was given a source term to account for internal energy generation.
### TABLE 2: Summary of Boundary Condition Settings

<table>
<thead>
<tr>
<th>Boundary Conditions</th>
<th>Setting</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Inlet</strong></td>
<td>Velocity=0.173 m/s</td>
<td>Calculated from volume flow rate and area of opening in quartz-tube.</td>
</tr>
<tr>
<td><strong>Outlet</strong></td>
<td>Outflow</td>
<td>Flow exit with unknown pressures and velocities.</td>
</tr>
<tr>
<td><strong>Coil Wall</strong></td>
<td>No Slip(^1)</td>
<td>To account for boundary layer on coil</td>
</tr>
<tr>
<td></td>
<td>(\varepsilon(T)=0.117^1)</td>
<td>Emissivity of platinum set according to expected average temperature.</td>
</tr>
<tr>
<td><strong>Tube in</strong></td>
<td>Shear stress=0</td>
<td>To account for plug-flow.</td>
</tr>
<tr>
<td></td>
<td>(\varepsilon=0.93^1)</td>
<td>Emissivity of quartz.</td>
</tr>
<tr>
<td></td>
<td>Semi-transparent(^1)</td>
<td>For radiation model.</td>
</tr>
<tr>
<td><strong>Inlet and Coil Ends</strong></td>
<td>T=290 K</td>
<td>The inlet air flow is at room temperature, and the coil ends are fixed at room temperature to account for effects of the large lead clips.</td>
</tr>
<tr>
<td><strong>Volume</strong></td>
<td><strong>Coil</strong></td>
<td>Source Term</td>
</tr>
<tr>
<td></td>
<td><strong>Air</strong></td>
<td>Participates in Radiation</td>
</tr>
<tr>
<td></td>
<td><strong>Quartz Tube</strong></td>
<td>Participates in Radiation(^1)</td>
</tr>
</tbody>
</table>

\(^1\) A setting was changed from the preliminary model.
TABLE 3: Summary of Model Settings

<table>
<thead>
<tr>
<th>Model</th>
<th>Settings</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>Pressure-based</td>
<td>Inlet velocity is due to a pressure gradient.</td>
</tr>
<tr>
<td></td>
<td>3D</td>
<td>Model drawing is three-dimensional.</td>
</tr>
<tr>
<td></td>
<td>Steady-state</td>
<td>During experiments, changes in electrical resistance were not recorded until they had stabilized at a steady state.</td>
</tr>
<tr>
<td></td>
<td>Implicit</td>
<td>Unknown temperature in each cell is dependent on unknown temperature of neighboring cells.</td>
</tr>
<tr>
<td>Energy Equation</td>
<td>On</td>
<td>Heat transfer is the main area of interest.</td>
</tr>
<tr>
<td>Radiation</td>
<td>Discrete ordinates</td>
<td>Solves radiative transfer equation for a finite number of discrete solid angles, for radiation heat transfer from the coil to air.</td>
</tr>
<tr>
<td>Viscous</td>
<td>Laminar</td>
<td>Re is extremely low in this application, less than 1 if calculated as a cylinder in cross-flow using wire diameter as characteristic length; laminar is the most appropriate option available. See discussion below.</td>
</tr>
</tbody>
</table>

With the boundary conditions input, the next step was to determine which models and restrictions should be applied (Table 3). The solver model was set to pressure-based, three-dimensional, steady-state, and implicit and the energy was set to run due to the heat transfer. The radiation model was set to run using discrete ordinates to account for the radiation heat transfer from the wire to the environment. Lastly, the viscous model was set to run for laminar flow, which was the best choice available for the low Reynolds number flow. The laminar flow setting coupled with all walls, except the coil wall, set to have zero shear stress was the best method to emulate the plug flow within the quartz tube. The upstream velocity profiles in FLUENT represent perfect plug flow as shown in Figure 6. Downstream of the flow disturbance due to the coil, the velocity remains fairly uniform across the diameter of the quartz tube. For comparison, velocity profiles measured with a hot-wire anemometer in the quartz tube are plotted in Figure 7. Figure 7 shows flat profiles +/- 13.8 percent across the diameter of the tube where the coil is located, similar to those shown in Figure 6 that were calculated with FLUENT.
FIGURE 6: FLUENT velocity contours in the flow around the coil and heated wire.

FIGURE 7: Measured velocity profiles near the coil.
4. RESULTS

For each model, the program was run with a source term accounting for a power input of 1 W up to 11 W. At each power input value, the temperature contours could be displayed, temperature as a function of position along the coil could be plotted, and the average temperature was reported. The temperature contours and plot for a power input of 9 W from the preliminary model are shown in Figures 8 and 9. The contour plots are useful to verify the model is working correctly, and the heat is being transferred downstream as expected. The temperature vs. position plot is important when we consider points of ignition and kinetics, because it shows the temperature range along the wire. This plot also shows that the leading sides of the coil are at higher temperatures than the sides. The ends of the coil are maintained at room temperature as set by the boundary conditions in FLUENT.

![Figure 8: Coiled wire and flow temperature contours with power set to 9 W.](image-url)
These plots, along with plots such as velocity and pressure plots that are available, are useful in determining if the models and parameters were defined correctly. However, the most useful output from FLUENT for our present purpose is the volume average integral report. The report provides the average wire temperature calculated by taking a weighted average by volume of the temperatures of the coil’s mesh elements. This temperature is comparable to the average temperature found experimentally. The temperatures calculated from each FLUENT model and those found experimentally are shown in Table 4 and are plotted in Figure 10.
### TABLE 4: Average Temperatures

<table>
<thead>
<tr>
<th>P (W)</th>
<th>E (W/cm³)</th>
<th>T_{exp} (K)</th>
<th>T_{prelim} (K)</th>
<th>ε of Pt</th>
<th>T_{rad} (K)</th>
<th>ΔT (K)</th>
<th>% Radiation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>517.99</td>
<td>344.77</td>
<td>363.66</td>
<td>0.04428</td>
<td>373.60</td>
<td>28.83</td>
<td>4.577</td>
</tr>
<tr>
<td>2</td>
<td>1035.97</td>
<td>414.83</td>
<td>427.21</td>
<td>0.05500</td>
<td>440.90</td>
<td>26.07</td>
<td>5.685</td>
</tr>
<tr>
<td>3</td>
<td>1553.96</td>
<td>476.85</td>
<td>483.99</td>
<td>0.06449</td>
<td>500.80</td>
<td>23.95</td>
<td>6.898</td>
</tr>
<tr>
<td>4</td>
<td>2071.94</td>
<td>532.36</td>
<td>535.75</td>
<td>0.07298</td>
<td>555.20</td>
<td>22.84</td>
<td>8.154</td>
</tr>
<tr>
<td>5</td>
<td>2589.93</td>
<td>582.64</td>
<td>583.52</td>
<td>0.07985</td>
<td>605.30</td>
<td>22.66</td>
<td>9.443</td>
</tr>
<tr>
<td>6</td>
<td>3107.91</td>
<td>628.68</td>
<td>628.00</td>
<td>0.08769</td>
<td>651.90</td>
<td>23.22</td>
<td>10.713</td>
</tr>
<tr>
<td>7</td>
<td>3625.90</td>
<td>671.24</td>
<td>669.69</td>
<td>0.09473</td>
<td>695.46</td>
<td>24.22</td>
<td>11.990</td>
</tr>
<tr>
<td>8</td>
<td>4143.89</td>
<td>710.80</td>
<td>708.94</td>
<td>0.10111</td>
<td>736.43</td>
<td>25.63</td>
<td>13.256</td>
</tr>
<tr>
<td>9</td>
<td>4661.87</td>
<td>747.57</td>
<td>746.05</td>
<td>0.10690</td>
<td>775.12</td>
<td>27.55</td>
<td>14.503</td>
</tr>
<tr>
<td>10</td>
<td>5179.86</td>
<td>781.53</td>
<td>781.26</td>
<td>0.11211</td>
<td>811.80</td>
<td>30.27</td>
<td>15.729</td>
</tr>
<tr>
<td>11</td>
<td>5697.84</td>
<td>812.37</td>
<td>814.75</td>
<td>0.11674</td>
<td>846.66</td>
<td>34.29</td>
<td>16.929</td>
</tr>
</tbody>
</table>

**FIGURE 10:** Average wire temperature vs. power plot.
In Table 4, $T_{\text{exp}}$ represents the average wire temperature determined experimentally, $T_{\text{prelim}}$ is the average wire temperature calculated assuming a high surface emissivity for the Pt, $T_{\text{rad}}$ is the average wire temperature calculated using $\varepsilon(T)$, and $\Delta T$ is the difference between $T_{\text{exp}}$ and $T_{\text{rad}}$. From Table 4 and FIGURE 10, it is clear that the temperature difference between the experimental values $T_{\text{exp}}$ and the preliminary model $T_{\text{prelim}}$ increases at low power inputs. The detailed model was run to try to explain the discrepancies at lower temperatures. It can be seen that the overall error between the detailed model $T_{\text{rad}}$ and the experimental values $T_{\text{exp}}$ is greater than the error between the preliminary model to the experimental data; however the detail model seems to have a constant offset of about 26.3K +/- 3.64K.

One issue that may be causing the discrepancies between the model and the experimental data may have to do with the experimental equipment. Although the power supply was rated for use at 0-60 A, the experiments ran at less than 5 A. The power supply is only accurate to 0.1 A, and for the 1 W experiment, the power supply was run at constant current less than 0.9 A. Inaccuracy in the power supply’s resolution at low range carries over into the determination of the wire temperature. Uncertainty in the experimentally obtained average temperatures is shown in Figure 11 for comparison with the calculated values, which lie close to the uncertainty bounds. For future experiments, a high precision power supply and measurement instrument has been purchased.
FIGURE 11: Temperature vs. power plot including experimental uncertainty.
5. SUMMARY AND CONCLUSIONS

Experimental data was recorded for an electrically heated platinum coil in cross flow. The average wire temperature was calculated as a function of power input. A three-dimensional drawing of the coil and the air around it was produced and meshed for finite element calculations in FLUENT. In FLUENT, material properties, boundary conditions and appropriate solver options were set. The program was run at each of 11 source terms that corresponded to 1-11 W power input, and the resulting average temperatures were recorded.

The preliminary FLUENT model results showed very good agreement with experimental results from 4-11 W. Below 4 W the difference in temperatures began to increase to a maximum difference of about 19 K at 1 W. The detailed FLUENT model results were consistently about 26K higher than the experimental data across the entire temperature range and did not show an increased deviation at low temperatures. This suggests that including the temperature variation of properties improved the model’s agreement with physical phenomena but that a consistent temperature offset remains. However, both the preliminary and detailed model results remain within the experimental uncertainty, which justifies a more accurate and precise power supply and volt meter rather than additional focus on modeling. These instruments have been purchased and are in use.

The model results also provide the temperature distribution along the coiled wire, an important consideration because of the sensitivity of surface reaction kinetics to temperature.

The temperature measurements permit the determination of the rate of heat generation at the surface due to catalytic reactions, important data for the development of practical igniters that achieve near-HCCI conditions in internal combustion engines.
6. ACKNOWLEDGEMENTS

This work was sponsored by a grant from the National Institute for Advanced Transportation Technology (NIATT), a University Transportation Center supported in part by the US Department of Transportation.
7. NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_p$</td>
<td>specific heat, J/(kg·K)</td>
</tr>
<tr>
<td>$E$</td>
<td>source term, W/cm$^3$</td>
</tr>
<tr>
<td>$g$</td>
<td>acceleration due to gravity, m/s$^2$</td>
</tr>
<tr>
<td>$k$</td>
<td>thermal conductivity, W/m</td>
</tr>
<tr>
<td>$n$</td>
<td>index of refraction</td>
</tr>
<tr>
<td>$P$</td>
<td>power, W</td>
</tr>
<tr>
<td>$p$</td>
<td>pressure, kPa</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature, K</td>
</tr>
<tr>
<td>$t$</td>
<td>time, s</td>
</tr>
<tr>
<td>$u$</td>
<td>velocity, m/s</td>
</tr>
<tr>
<td>$x$</td>
<td>volume percentage</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>emissivity</td>
</tr>
<tr>
<td>$\mu$</td>
<td>dynamic viscosity, kg·m/s</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>viscous dissipation function W/m$^3$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>equivalence ratio</td>
</tr>
<tr>
<td>$\rho$</td>
<td>density, kg/m$^3$</td>
</tr>
</tbody>
</table>

SUBSCRIPTS

- $r$: radial direction
- $z$: axial direction
- $\theta$: azimuthal direction
8. REFERENCES


