SIMULATION MODEL OF EXOTHERMIC REACTIONS FOR HEAT LOSS MITIGATION ON STEAM PIPES

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Abstract

Applying exothermic reaction to steam pipes to mitigate heat loss is an idea that is yet to be explored. By using simulation modeling, this paper focuses on gathering theoretical data to serve as the baseline for the actual application. The initial condition of the simulations was set-up to emulate the actual environment around steam pipes. The data gathered were able to provide enough theoretical evidence showing that applying exothermic reaction causes a tremendous increase in the temperature of the steam.

Keywords: Thermodynamics, Heat Transfer, Steam Power Plant, Enthalpy, Bond Energy

Introduction

A crucial role in designing vehicles, buildings, power plants, electronic devices, refrigerators and bridges among other things is played by understanding the mechanism of heat transfer (Cengel, 2003). One of the most effective methods for heat transfer especially in power generation is by utilizing steam pipes. However, unavoidable heat losses affect the steam pipe's efficiency and in effect, causes more fuel consumption especially in steam power plants. As mentioned by Anand et al. (2010), from the end user's side, the energy is reduced by heat loss that usually happens on the surfaces of bare steam pipes causing an additional toll on the boilers. On his work, Stevens (2010) mentioned that the amount of energy lost could be ten times greater than the energy being delivered through steam pipes if proper insulation is not observed. However, a study of McNabb & Weir (1980) concluded that though the thermal capacity of the pipes may increase with insulation, yet under an intermittent condition, it resulted in more energy loss. Other researchers conducted studies on ways in insulating steam pipes by utilizing different materials such as Bansal et al. (2010) which used cement, mineral wool, and lead with different thicknesses to insulate steam pipes and mitigate heat loss.

This paper aims to introduce a new idea to mitigate heat loss in steam pipes other than insulation. The idea is to apply exothermic reaction to steam pipes and add the heat produced by this reaction to the heat carried by the pipes. Theoretically, by doing such will not only mitigate the heat loss but also prevent it from happening. Exothermic reaction as defined by Helmenstine (2016), is a chemical reaction that releases energy by light or heat. However, this paper focuses primarily on the simulation of the reaction rather than its actual application. Simulation of the molecular combination and chemical reaction of the main elements that will cause the exothermic reaction is necessary to serve as baseline data for the actual application. The simulation aims to show the best possible molecular combination of the elements that cause the highest temperature increase and the longest time duration for the exothermic reaction. The reaction produced is based on the principle of solid combustion. Klippenstein (2016) mentioned that through thousands of reactions, chemical conversion of hundreds of species is treated by chemical modeling of combustion. In this paper, the simulation parameters are based on the actual environment of steam pipes.

Shown in Figure 1 is the conceptual framework of the study. The combination of elements necessary to produce an exothermic reaction will be varied to find its best possible combination resulting to an exothermic reaction which gives off the highest temperature increase with the longest time duration.

Figure 1. Conceptual Framework
Methods

The study used an experimental design, particularly simulation modeling. The experimental criteria measured were the rise in temperature, time duration of the exothermic reaction, and the molecular combination of N2 and O2. In the study of Klippenstien (2016), he cited that the level of accuracy of the parameters that make up the chemical model naturally dictates the fidelity of the simulations. Therefore, all simulation parameters were based from previous studies and public knowledge. It is common knowledge that the standard mixture of air consists of 78% nitrogen molecules and 21% oxygen molecules while the remaining 1% is composed of other gases like argon. The simulation set-ups were based on this data having N2 as constant at 78% for the first set-up while varying the O2. The same reason went for the second set-up when O2 molecules were set as constant to 21 while varying N2.

The simulation set-ups were based on the principle that it is preferable and easier to add nitrogen or oxygen molecules rather than extract it from the air composition. In this paper, set-ups were considered to have used 100 molecules of air for the exothermic reaction. For both set-ups, charcoal geometry was set at 6 x 6. Thus, the maximum number of oxygen molecules is only limited up to 36. On the other hand, the minimum number of O2 was limited to 21 since its standard molecular composition in the mixture of air is 21%. To create a variety of range for the trials, other values for O2 were randomly assumed from the numbers between its minimum and maximum values while N2 was set as constant at 78%. The same process was done for the second set-up, the only difference is, this time the O2 was the one set as constant at 21 while varying N2. Figure 2 shows an initial set-up before the exothermic reaction happened. The initial conditions for the simulation were based on the following assumptions.

Assumptions:
1. The initial temperature is set to 374 o C. The critical level of the temperature of the steam is 374 o C (Haroon, 2017). At this temperature, no matter how much pressure is applied, the steam cannot be liquefied.
2. The energy release or bond energy of carbon dioxide is set to 800 0C (Clark, 2013).
   This is the amount of potential chemical energy released in the burning reaction.
3. Charcoal geometry is set to 6x6.
   It determines the shape of the cluster of carbon atoms.
4. One tick is equivalent to 4 seconds.
   Ticks correspond to the time duration in the simulation. However, the length of one (1) tick in the simulation is equivalent to four (4) seconds. This was found out by using stopwatch/timer to convert the duration of ticks to real-time values.

Measured Parameters:
1. Number of molecules of N2 and O2.
2. Increase in temperature
3. Duration of the exothermic reaction

After the initial condition for the simulation was set-up, the simulation was run ten (10) times for every variation of the N2 and O2 molecules. Figure 2 illustrates the initial set-up of the simulation.

![Figure 2. Initial Set-up of the Simulation](image-url)
Model Specification

This study used an agent-based simulation software called Net Logo 5.3 (2013) principally authored by Uri Wilensky, specifically, the Connected Chemistry-Solid Combustion (2007) that shows the chemical kinetics of the combustion reaction for burning charcoal. Energy is released (exothermic reaction) when charcoal undergoes combustion. This is due to the chemical reaction that happens when the oxygen (O2) found in the air reacts to the carbon (C) atoms that are mostly made of charcoal in which this reaction produces carbon dioxide (CO2). This chemical reaction is represented as follows:

\[ C + O_2 \rightarrow CO_2 \]

where CO2 is the product produced by the reaction caused by reactants C and O.

Charcoal was modeled in the form of a block solid of 100% pure carbon in this model. The surrounding gas was modeled as oxygen and nitrogen. However, the model treats nitrogen as an inert gas that does not react with either oxygen or carbon aside from the fact that molecular nitrogen and oxygen may combine to form a nitric oxide at high temperatures. Also, chemical reactions to form N4, which is called nitrogen diamond can happen at high temperatures and pressures when two N2 molecules react. Neither of these reactions was represented in this model.

Results and Discussion

Data on Table 1 implies that setting the N2 molecule as constant at 78 while varying the O2 molecules resulted in a variety of temperature increase. Setting the oxygen molecules to 36 produced an exothermic reaction for which the occurrence lasted the longest and gave off the highest temperature rise among others. An increase of 243 OC, which was the highest for this set-up, can be of great assistance in mitigating heat loss from the steam pipe.

Table 1. Measure of time duration and temperature increase of the exothermic reaction with constant N2 molecules and variable O2 molecules

<table>
<thead>
<tr>
<th>Number of O2 Molecules (mols)</th>
<th>Average Time When Reaction Started (s)</th>
<th>Average When Reaction Ended (s)</th>
<th>Average Time Duration of the Reaction (s)</th>
<th>Highest Increase in Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>21</td>
<td>3.15</td>
<td>139.65</td>
<td>136.50</td>
<td>163</td>
</tr>
<tr>
<td>26</td>
<td></td>
<td></td>
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<tr>
<td>31</td>
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<tr>
<td>36</td>
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<td></td>
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<td></td>
</tr>
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<td>3.15</td>
<td>139.65</td>
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<td>163</td>
</tr>
</tbody>
</table>

Shown in Figure 3 is a 3-dimensional graph indicating the relation of all the measured criteria for the first set-up. For this set-up, all values given to the O2 molecules showed a significant increase in temperature caused by the occurrence of an exothermic reaction. It is noticeable that there is a directly proportional relationship between the increase in molecules of O2 and the temperature increase.
The tabular data from Table 2 shows that by setting the O2 molecules as constant at 21 while varying the N2 molecules did not give as much temperature increase and time duration for the exothermic reaction compared to the first table.

Table 2. Measure of time duration and temperature increase of the exothermic reaction with constant O2 molecules and variable N2 molecules

<table>
<thead>
<tr>
<th>Number of N2 Molecules (mols)</th>
<th>Average Time When Reaction Started (s)</th>
<th>Average When Reaction Ended (s)</th>
<th>Average Time Duration of the Reaction (s)</th>
<th>Highest Increase in Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>78</td>
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<td>139.65</td>
<td>136.50</td>
<td>163</td>
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</tr>
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</tr>
</tbody>
</table>

The 3-dimensional graph on Figure 4 illustrates that by varying N2 molecules while having the O2 at constant, still showed good results in increasing the temperature of the gases. However, an inversely proportional relationship between the number of N2 molecules and increased temperature were observed. Assuming this pattern continues, increasing the number of N2 molecules will only result to a much lower temperature increase.
Illustrated in Figure 5 is the simulation of the on-going exothermic for the set-up where N2 molecules were set to constant at 78 while O2 was varied (in this case O2=36). This set-up gave the longest time duration of the exothermic reaction at the same time gave off the highest increase in the temperature of the gases.

![Exothermic Reaction Simulation](image)

**Figure 5. Exothermic Reaction when O2=36 and N2=78**

**Conclusions**

Application of exothermic reaction causes a noticeable increase in temperature of gases. The energy from exothermic reaction that is usually transferred as heat energy causes the reaction mixture and its surroundings to get hotter ("Exothermic reaction," 2014). According to Xi Lu, et al. (2017), increasing the kinetic energy by increasing the temperature allows greater movement in the gas particles, which in result causes an increase in temperature to its surroundings. Researchers used the simulation model to simulate the effects on the temperature increase and time duration of an exothermic reaction when the main components for the reaction are altered and adjusted. Simulation results revealed that altering the main components responsible for the occurrence of an exothermic reaction has tremendous effects on its temperature increase and time duration. Experimental data showed that the maximum temperature increase acquired from the exothermic reaction is 243°C. The simulation revealed that to produce the desired exothermic reaction causing this temperature increase, it needs to have 78 N2 molecules and 36 molecules of O2. However, utilizing air (78% nitrogen molecules and 21% oxygen molecules) for the exothermic reaction does not provide enough oxygen molecules for the desired mixture thus, injecting an additional of 15 O2 molecules per 100 molecules of air is necessary.

**Acknowledgments**

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References


