Life Cycle Analysis of a Ceramic Three-Way Catalytic Converter

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ABSTRACT

The life cycle analysis compares the environmental impacts of catalytic converters and the effects of not using these devices. To environmentally evaluate the catalytic converter, the emissions during extraction, processing, use of the product are considered. All relevant materials and energy supplies are evaluated for the catalytic converter. The goal of this life cycle is to compare the pollutants of a car with and without a catalytic converter. Pollutants examined are carbon monoxide (CO), carbon dioxide (CO_2), hydrocarbons (HC), and nitrogen oxides (NO_x). The main finding is that even considering materials and processing, a catalytic converter decreases the CO, HC and NO_x pollutant emissions. The CO_2 emissions are increased with a catalytic converter, but this increase is small relative to the overall CO_2 emissions. The majority of catalytic converter pollutants are caused by the use phase, not extraction or processing. The life cycle analysis indicates that a catalytic converter decreases damage to human health by almost half, and the ecosystem quality damage is decreased by more than half. There is no damage to resources without a converter, as there are no materials or energy required; the damages with a converter are so small that they are not a significant factor. Overall, catalytic converters can be seen as worthwhile environmental products when considering short term effects like human health effects of smog, which are their design intent. If broader environmental perspectives that include climate change are considered, then the benefits depend on the weighting of these different environmental impacts.

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Table of Contents

List of Figures

List of Tables

List of Equations

1.0 Introduction

Air pollution is a very important topic in current society as it affects the quality of human life and the environment. Any substance that is introduced into the atmosphere that has damaging effects on the environment and living species is considered air pollution [1]. The sources of air pollution include, but are not limited to, transportation, power plants, and human activities that involve the burning of fossil fuels; an example of a human activity that causes air pollution is heating and cooling a home or workplace [1]. The emissions created by an individual vehicle are generally low, compared to many other pollutant sources; however, emissions from millions of vehicles add up. The personal vehicle is the single greatest contributor to air pollution, by mass, in the United States [2].

1.1 The Catalytic Converter

In order to move a car, power is generated in the engine by burning fuel. The combustion of fuel creates emissions. Gasoline, which is the fuel source for 98 percent of passenger cars, is a mixture of hydrocarbons (HC) [3]. These are compounds that contain hydrogen and carbon atoms. In a "perfect" engine, all of the hydrogen and carbon in the fuel would be converted to water vapor and carbon dioxide, respectively, by combustion with the oxygen from the air. The nitrogen from the air would not be affected in the combustion process [2]. This can be seen in Equation 1.1 below. However, engines are not "perfect", and the combustion process creates other chemical byproducts which contribute to air pollution. This can be seen in Equation 1.2 below [Environmental Protection Agency, EPA National Vehicle and Fuel Emissions Laboratory. (n.d.). *Automobile emissions: An overview* (EPA 400-F-92-007). Retrieved from Office of Mobile Sources website: http://www.epa.gov/otaq/consumer/05-autos.pdf]. (Used under fair use, 2012).

“Perfect” Engine: (1.1)
Fuel (hydrocarbons) + Air (O_2 and N_2) → Carbon Dioxide (CO_2) + Water Vapor (H_2O) + Unchanged Nitrogen (N_2)

Typical Engine: (1.2)
Fuel (hydrocarbons) + Air (O_2 and N_2) → Unburned Hydrocarbons (gases and solid particulate matter) + Carbon Dioxide (CO_2)
+ Water Vapor (H_2O) + Nitrogen Oxides (NO_x) + Carbon Monoxide (CO)

1.1.1 Exhaust pollutants

When fuel molecules do not burn, or partially burn during the combustion process, hydrocarbon emissions are created [2]. Reacting in the presence of NO_x and sunlight, hydrocarbons form ground-level ozone (O_3). A major contributor to smog, ozone is the most widespread and hard to control urban air pollution problem. It can be an eye irritant, cause lung damage, and aggravate respiratory problems. Hydrocarbons themselves can be toxic and potentially carcinogenic. Benzene (C_6H_6) is an example of a hazardous hydrocarbon. This pollutant can prevent proper production of red blood cells and the loss of white blood cells [4]. Toluene (C_7H_8) is another common hydrocarbon emission that can cause asthma [5].

Due to high pressures and temperatures occurring in the combustion process, oxygen and nitrogen react to form various nitrogen oxides [2]. NO_x contributes to the formation of ozone and acid rain. Ozone is the primary component of smog, and therefore NO_x creates similar impacts to hydrocarbons. Nitrogen oxides are potentially toxic to plants, as they can reduce growth and damage leaves [6]. These pollutants are also known to irritate lungs and cause respiratory infections.

Carbon monoxide is created when carbon only partially oxidizes [2]. CO is dangerous to health as it decreases the flow of oxygen in the bloodstream. It can impair several sites within the body, but has the greatest effect on the organs with the highest oxygen requirements (brain, heart, etc) [7].

Carbon dioxide is the largest emission by mass from both perfect and real engines. Historically, it has not been considered an environmental impact and there are currently no emission standards for it. However, in the past few decades, CO_2 has been viewed as a greater environmental concern. While CO_2 is not a short term threat to human and environmental health, it is a greenhouse gas. This means it traps the heat from the earth and is a contributor to global warming potential [2].

1.1.2 Environmental Protection Agency Regulation History

The Environmental Protection Agency (EPA) established the Clean Air Act, which was first enacted in 1970, to set vehicle air emission standards throughout the years [2,3]. Table 1.1 below provides the emission standards for a light passenger car from 1968 to 1994. The standards set in 1994 are the current emission standards for an individual light passenger car. The values are given in grams per mile. These values are different for trucks and sport utility vehicles.

Table 1.1: American emission standards (gram/mile) set by federal legislation [Degobert, P. (1995). *Automobiles and pollution*. (2 ed., pp. 124-129). Warrendale, PA: Society of Automotive Engineers, Inc.]. (Used under fair use, 2012).

Year	Carbon monoxide	Hydrocarbons	Nitrogen oxides
	Light Passenger Cars		
1968-69	51	6.3	-
1970-71	34	4.1	-
1972	28	3.0	-
1973-74	28	3.0	3.1
1975-76	15	1.5	3.1
1977-79	15	1.5	2.0
1980	7.0	0.41	2.0
1983	3.4	0.41	1.0
1994	3.4	0.25	0.4

The Clean Air Act of 1970 set strict emission regulations that would be enforced starting in 1975 [2]. The emission regulations can be seen in Table 1.1 above. From 1968 to 1972, the nitrogen oxide emissions were not measured, and are therefore represented by a dash. From 1970 to 1974, car manufacturers attempted to decrease CO and HC emissions; however, despite these attempts to meet the regulations by adjusting the engine alone, the catalytic converter was introduced in order to reach the standards. The first generation was known as two-way catalytic converters because they converted hydrocarbons and carbon monoxide into water vapor and carbon dioxide.

The introduction of the catalytic converter also indirectly decreased ambient lead levels [2]. Because the catalysts in catalytic converters are poisoned and inactivated by lead, unleaded gasoline was widely introduced across the United States. This helped to lessen human health and environmental concerns due to lead pollution. Once a human ingests lead, it distributes throughout the body, in the blood, and accumulates in the bones [9]. The most common health effects from lead are neurological effects in children and cardiovascular effects in adults, such as high blood pressure and heart disease. In the environment lead accumulates in soils and sediments. Ecosystems near point sources of lead can have adverse effects, such as losses in biodiversity, changes in community composition, decreases in plant and animal growth and reproduction rates, and neurological effects in vertebrates [9].

In 1977, the Clean Air Act was amended to more strictly regulate emissions [10]. As per the request of automakers, the standards were delayed until 1980 and 1981. The emission regulations for the amendment can also be seen in Table 1.1 above. The new HC and CO standard was put into effect in 1980. A new standard to regulate NO_x also went into effect in 1981; this can be seen in Table 1.1 by the year 1983. The second generation technology was known as the three-way catalytic converter because it managed all three primary vehicle emissions (HC, CO and NO_x).

1.1.3 Design and Materials

Figure 1.1 below depicts two ceramic monoliths, which are the key to the catalytic converter; the first monolith contains the reduction catalyst [11]. The second monolith contains the oxidation catalyst. A two-way converter only employed the second monolith, while both make up the three-way converter. The Lambda probe was another improvement to the catalytic converter that came about with the three-way converter [11]. A control system monitors the exhaust stream by the way of the oxygen sensor, the Lambda probe. The system controls the fuel injection system, which allows the engine to run as efficiently as possible while producing the least emissions.

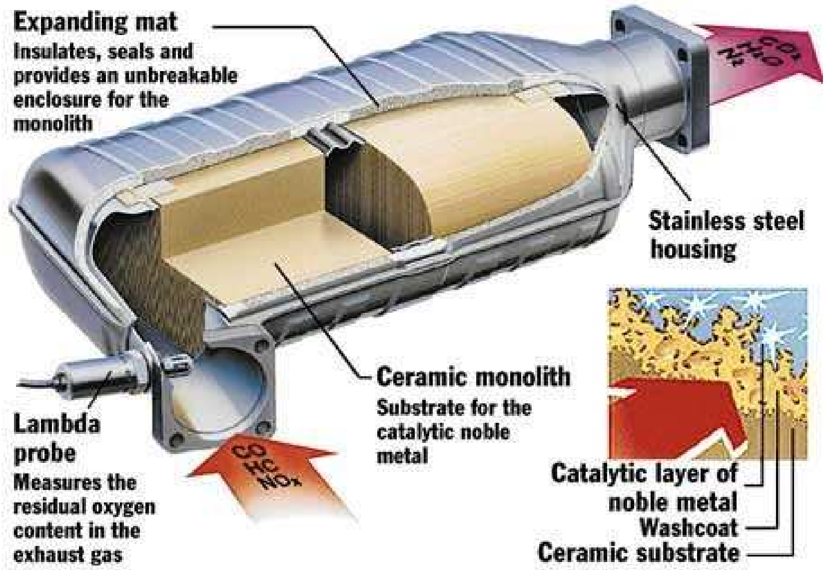

Figure 1.1: Schematic of a catalytic converter [*Motor vehicle emission controls: Technologies*. (n.d.). Retrieved from http://www.air-quality.org.uk/25.php]. (Used under fair use, 2012).

Figure 1.2 below provides the typical process flow for the creation of a catalytic converter. In the production, the catalytic converter is processed in three phases. The boxes outlined in red indicate the processes that will be considered in scope for this analysis.

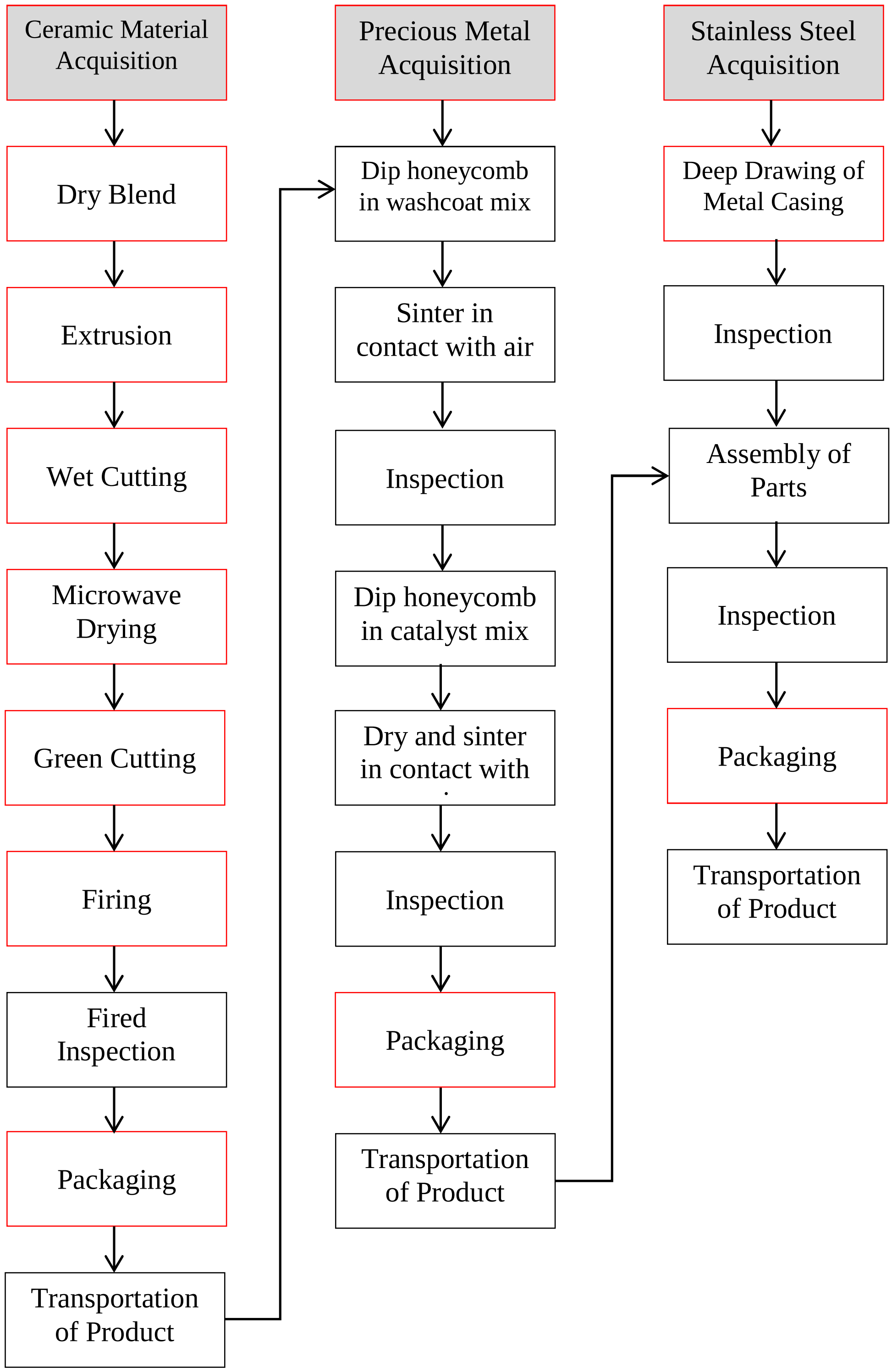

Figure 1.2: Process flow diagram

The ceramic component of the catalytic converter is formed from a honeycomb structure made of extruded cordierite, as seen in Figure 1.3 below [12]. Cordierite ($2MgO-2Al_2O_3-5SiO_2$) is appropriate for application in automotive exhaust because it has a relatively low thermal expansion, which is needed for thermal shock resistance. The coefficients of thermal expansion generally fall in the range of $0.7 – 1.0 \cdot 10^6$ per degrees Celsius from 25° – 1000° C [12]. With a melting point of 1500 – 1700 °C, this material is also a refractory; this allows cordierite to operate at high temperatures [12, 13]. Cordierite is inert to the catalysts and coatings that are used. This material can also be engineered to provide other features, such as, open porosity and good mechanical strength [12]. The tensile strength and fracture toughness of cordierite is 48 – 53 MPa and 2 – 3 $MPa \cdot m^{0.5}$, respectively [13].

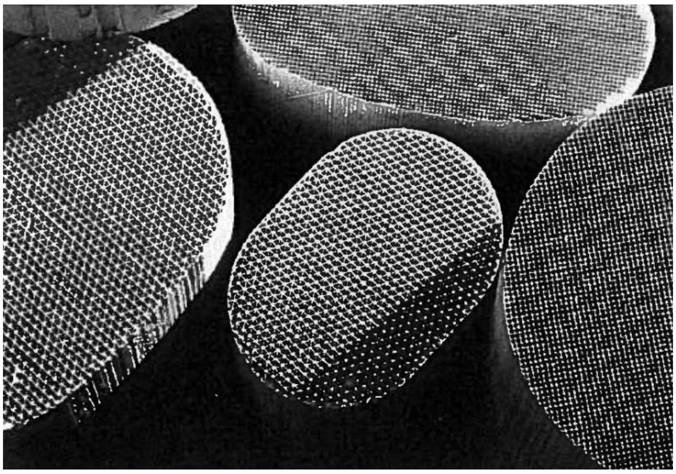

Figure 1.3: Cordierite honeycomb structures [Lachman, I., Bagley, R., & Lewis, R. (1981). Thermal expansion of extruded cordierite ceramics. *Ceramic Bulletin, 60*(2), 202-205.]. (Used under fair use, 2012).

Each ceramic monolith is coated with a washcoat and a catalyst coating made with a precious metal. The washcoat is made of alumina and/or silica and a rare earth metal oxide such as cerium oxide [14]. The cerium oxide can release or capture oxygen in the exhaust [15]. It can also work with the other catalytic materials to aid in emission conversion. It is applied in order to coat the smooth ceramic substrate walls. The washcoat helps to provide a much larger surface area by forming a rough and irregular surface. The greater surface area allows for a larger number of sites for the precious metals to coat to [14]. Precious metals are used for the catalytic coating; platinum and/or palladium are used for the oxidizing catalyst, and rhodium is used for the reducing catalyst. The platinum and/or palladium are responsible for dissociating the hydrocarbons and carbon monoxide molecules [16]. When the hot gases encounter the platinum or palladium particles, they react to form water and carbon dioxide molecules. The platinum and/or palladium molecules lower the energy barrier that slows down the conversion of the emissions.

Surrounding the coated ceramic monoliths is an expanding mat. This mat insulates and protects the ceramic monoliths. Finally, the entire structure is encased by a stainless steel housing [11]. Type 409 ferritic stainless steel is commonly used for this structure because it provides corrosion and oxidation resistance with ease of fabrication [17, 18].

The two-way converter is also known as an oxidation catalyst [18]. The metal catalyst (platinum and/or palladium and rhodium) is used to super heat the HC and CO gases. The heat converts the HC and CO gases by oxidizing them with oxygen. Equations 1.3 and 1.4 below give the oxidation equations for CO and HC gases. Since there are various forms of hydrocarbons, Equation 1.5 below gives the oxidation equation for benzene (C_6H_6), which is a very common form of hydrocarbon [19].

$$2CO + O_2 \rightarrow 2CO_2 \tag{1.3}$$

$$4HxCy + 5O_2 \rightarrow 2xH_2O + 4yCO_2 \tag{1.4}$$

$$2C_6H_6 + 15O_2 \rightarrow 12CO_2 + 6H_2O \tag{1.5}$$

The three-way catalytic converter is also known as the reduction-oxidation converter [11]. Since catalytic converter technology, up until this point, did not regulate NO_x, an additional reduction catalyst was created; this was used with the oxidation catalyst in the two-way converter. The reduction catalyst uses the precious metals to help reduce NO_x emissions. Rhodium is responsible for dissociating the nitrogen oxide molecules. In the same manner as platinum and palladium, when the hot gas encounters the rhodium molecules, the nitrogen and oxygen atoms separate on the metal's surface. These atoms recombine into nitrogen and oxygen molecules [16]. Equations 1.6 and 1.7 below give possible reduction equations of NO_x.

$$2NO \rightarrow N_2 + O_2 \tag{1.6}$$

$$2NO_2 \rightarrow N_2 + 2O_2 \tag{1.7}$$

In the creation of a catalytic converter, many steps must be taken, including raw material gathering and various forms of processing. After the converter is created, it goes through a period of use, in which pollutants are converted to less harmful substances. Once the converter is no longer in use, it is disposed of. Parts of the catalytic converter can be recycled, such as the metals, and the other parts are landfilled, such as the ceramic monoliths. In each of these steps, materials, energies and wastes are necessary. While the use and recycling phases offer positive environmental impacts, the raw materials, processing and disposal steps create negative impacts. In order to determine the environmental impact of the catalytic converter over its whole life cycle, a life cycle analysis (LCA) is used. This analysis will compare the positive to the negative environmental impacts of a catalytic converter over the whole life cycle in order to better assess this product from an environmental perspective.

1.2 Life Cycle Analysis

Life cycle analysis (LCA) is a method of assessing the environmental impact of a product over its lifetime [20]. The lifetime of most products typically includes four phases: extraction of raw materials, manufacturing/processing of the raw materials, use and disposal of the product. Environmental impacts from each phase can be estimated to provide an overall impact of the product's life. This evaluation provides a more accurate depiction of the environmental trade-offs that come with the selection and design of a product. Figure 1.4 below depicts the phases and the inputs and outputs that are associated with an LCA [20]. The inputs are the raw materials and energies that are used in the various life cycle phases. The outputs are any emissions or byproducts created from any of the phases. The system boundary is the box around the life cycle phases. It defines the limitations of analysis, including what will and will not be considered [20].

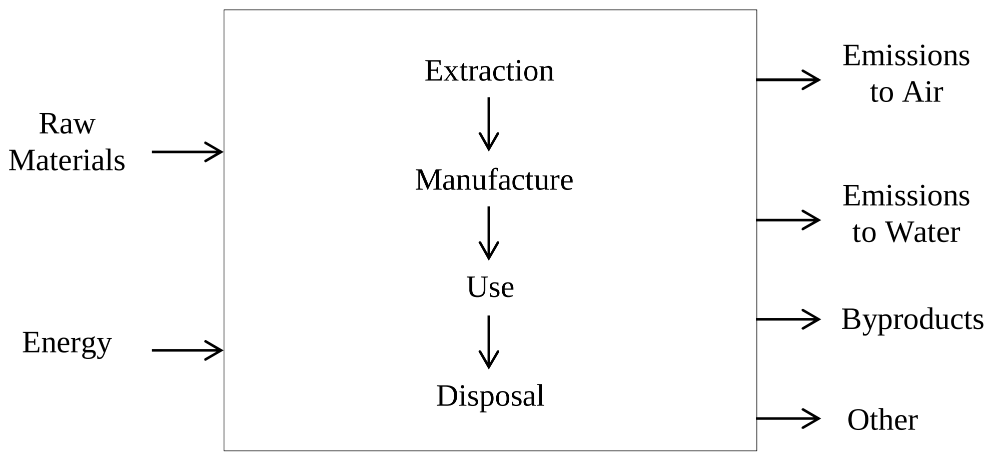

Figure 1.4: Life cycle analysis phases and inputs and outputs [Curran, M. A. U.S. Environmental Protection Agency, Office of Research and Development. (2006). *Life cycle assessment: Principles and practice* (EPA/600/R-06/060). Reston: Scientific Applications International Corporation (SAIC).]. (Used under fair use, 2012).

1.2.1 Life Cycle Inventory

A life cycle inventory (LCI) is a collection of quantitative inputs and outputs for the entire life cycle of a product. This step of the LCA is basically an inventory of all relevant energies, materials, emissions and wastes [20]. An LCI is an important part of an LCA because it provides the evaluation basis for comparing environmental impacts or potential improvements. The LCI can help to compare products or processes while considering environmental factors during material selection and design. The results of an LCI provide a quantitative list of pollutants released to the environment as well as the total amount of energy and raw materials consumed. There are four basic steps of a life cycle inventory defined by the EPA [20]. In the first step of an LCI, a flow diagram of the product being evaluated is developed. This diagram will define the inputs and outputs in the system. The system is defined by the system boundaries. The more complex the flow diagram, the more accurate the results will be; conversely, the more complex the flow diagram, the more time and resources will be required. The second step of an LCI is to develop a data collection plan and acquire the necessary data. This step ensures that the data collection is planned, organized and of the quality and accuracy desired. The collection must include any and all data required for the entire LCA. It should correspond to the flow diagram developed. The third step of the LCA is the impact assessment (LCIA) which translates LCI input and outputs to specific environmental impacts based on the best available science. The final step of an LCIA is the evaluation and documentation of the LCI results. The explanation of the LCA should explicitly define the system, assumptions, inputs, and resulting outputs.

1.2.2 Goal

The goal of the thesis is to gather and assess existing data that will be used to develop a model of the life cycle of a ceramic three-way catalytic converter. More specifically, the goal is to compare the embodied energy and production of pollutants developed during extraction, manufacturing and disposal to prevention of pollutants during use. The research will compare the pollutants phase by phase; for example, the pollutants of materials can be compared to those of manufacturing to show which phase contributes more to the overall pollution. This comparison can also provide insight on which phase could use the most improving if trying to decrease the pollution to the environment. The same can be done within each phase to show which portion or step of the phase can use the most improving.

1.2.3 Tasks

In order to accomplish the goal stated above, the following key tasks that must be completed:

1. Determine and set a boundary for the research. This boundary will set what will and what will not be included in the analysis.
2. Collect information on the materials and processing required to create a catalytic converter. Information is also needed on the emissions during use for both a car with and without a catalytic converter.
3. Create and develop two life cycle models; one for the entire life of a catalytic converter, and one for the use phase of a car without a catalytic converter.
4. Run model and analyze results to determine the environmental impact of a car with a catalytic converter compared to a car without a catalytic converter.

The first life cycle model is a car without a catalytic converter. In this model, only the emissions during the use phase will be analyzed. The second life cycle model is a car with a catalytic converter. This model will analyze the extraction and processing of raw materials, manufacturing of the catalytic converter and the emissions during the use phase. The car itself is not included in this analysis since all of its environmental impacts are the same except for the catalytic converter and emissions.

1.2.4 Scope

The scope of this project is defined by the function of a catalytic converter, the functional unit, and the system boundaries. The function of a catalytic converter is to convert engine exhaust from hazardous to less hazardous chemicals. The functional unit, which serves as the basis of comparison, is the average lifetime of a catalytic converter for a typical light passenger car. The guaranteed service lifetime of this catalytic converter is 80,000 miles [21]. A specific vehicle was chosen in the research for ease and accuracy of data; however, this methodology could be applied to any vehicle to obtain similar results.

The system boundaries include the inputs and outputs of energy, materials, and transportation for all phases of the LCI. The emissions that will be primarily analyzed in this study are carbon monoxide, carbon dioxide, nitrogen oxides, and hydrocarbons. The system boundaries exclude all capital goods (such as the existing manufacturing equipment), human labor and incidentals. These categories are excluded because over time and divided between all of the components created, their effect becomes negligible. The Society of Environmental Toxicology and Chemistry (SETAC) guidelines for life cycle assessment state that inputs of a process do not need to be included in the LCI if (i) they are less than 1% of the total mass of the processed materials or product; (ii) they do not contribute significantly to a toxic emissions; and (iii) they do not have a significant associated energy consumption [22]. Similarly, the organic binders used during ceramic processing are out of scope. The binders are not included because they are highly proprietary and likely fall within the SETAC guidelines. To include them would require unreliable information and estimation, therefore compromising the integrity of this report. The oxygen sensor is not considered a part of the catalytic converter. While it functions in conjunction with a catalytic converter, it is not an integral part of the component, and is manufactured separately. The energy necessary to weld the stainless steel canister is negligible. Compared to the rest of processing, there is very little energy used during welding since the area welded is very small. The plastic used during packaging is negligible. Only a small amount of plastic is used during packaging for an entire box, but divided between the multiple components, even less is required. Fuel mileage and car performance will also be excluded from the research, due to the lack of impact the catalytic converter has on them (Dr. Al Kornhauser, Virginia Tech, personal communication) [23]. The expanding mat that lies between the ceramic monolith and the stainless steel casing will be left out of scope. The composition of the mat is proprietary, and therefore any estimation would also be inaccurate. During manufacturing, the processing energies associated with applying the metal washcoat and catalysts are not included in this analysis. The methodology and energies associated with these processing steps are proprietary and no acceptable estimates could be found in the literature. The plastic packaging materials and the paper filler are left out of scope as they have very small masses compared to the cardboard box, and can be considered insignificant. Finally, anything that falls into the aforementioned categories is depicted in the scope and boundary figure below. Everything in the outside box is excluded in the scope of the project, while the inner box is included in the study.

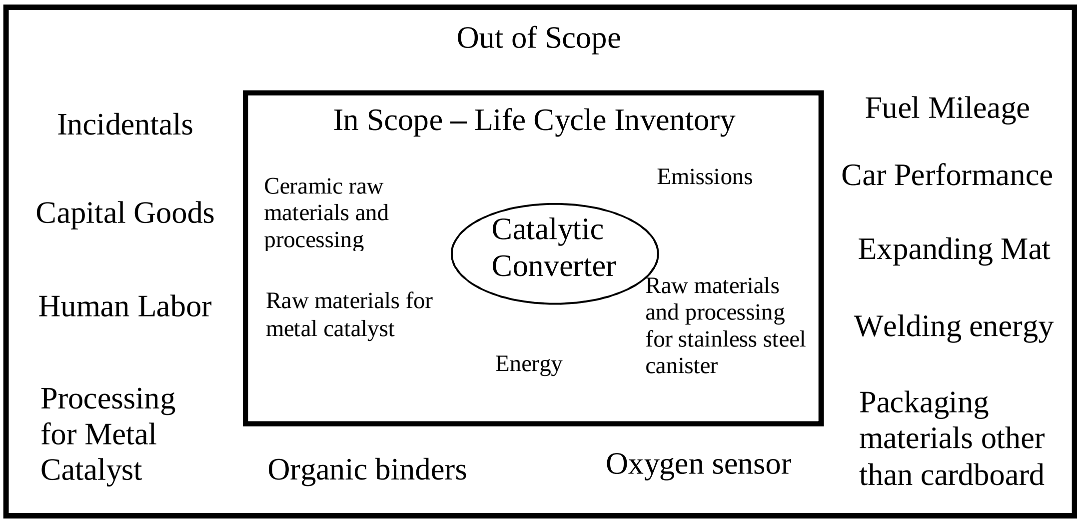

Figure 1.5: Schematic of project scope

1.2.5 Assumptions

It is important to list any and all assumptions for an LCA since they strongly influence the results. This helps to make processes and decisions explicit to the reader. Below is a list of the assumptions used in this life cycle.

- The catalytic converter is manufactured in southwest Virginia. To allow for accurate production energy mix, all of the electricity entered into SimaPro will use the southwest Virginia energy mix provided by American Electric Power.
- The catalytic converter is manufactured in three phases at different manufacturers (ceramic, catalyst coating, and steel housing).
- The cordierite processing energies are the average of the magnesia brick processing energies. This assumption will be tested with sensitivity analysis by taking 50% and 75% of the average drying and firing energies. Magnesia is fired at higher temperatures than cordierite. Magnesia brick is fired between 1500°C – 1750°C, while cordierite is usually

fired around 1400°C [12, 24]. This suggests that MgO uses greater energy; therefore the analysis will look at decreasing the energy.

- Platinum is solely used for the oxidation catalyst. The use of palladium or a mix of the two metals will be tested with a sensitivity analysis.
- The precious metal coating is a mix of platinum, rhodium and lanthanum oxide, and it will be used on both substrates according to Patent Number 4,624,941 [25].
- Alumina is solely used as the bulk of the washcoat. Silica and a mix of the two materials will be tested with a sensitivity analysis.
- Microwave drying is used to draw water out of the wet extruded ceramic (confidential, ceramic manufacturing company, verbal communication). This assumption will be tested with a sensitivity analysis of using conventional drying instead.
- Conventional firing is used (confidential, ceramic manufacturing company, verbal communication). Microwave firing will be tested with a sensitivity analysis.
- Twelve ceramic substrates are placed in a cardboard box for shipping (at the ceramic and catalyst coating facilities) (confidential, ceramic manufacturing company, verbal communication).
- One catalytic converter is placed in a cardboard box for shipping (at the steel housing facility) (Matthew Bentel, Harrisonburg Honda, verbal communication).
- The converted nitrogen, oxygen and water vapor do not pose a risk to the environment compared to carbon dioxide, carbon monoxide, hydrocarbons and nitrogen oxides and are therefore not modeled as emissions.
- The catalytic converter is not broken or does not malfunction over time.

2.0 Life Cycle Analysis Method

In order to complete the life cycle analysis, a collection of all materials, energies, emissions and other data is required. The life cycle is conducted using the software program SimaPro 7.3. SimaPro, developed by PRé Consultants, is a leading life cycle analysis software [26]. This program offers standardization but also flexibility when modeling or designing. SimaPro is used for various applications, including:

- Carbon footprint calculation
- Product design and eco-design
- Environmental Product Declarations (EPD)
- Environmental impact of products or services
- Environmental reporting (GRI)
- Determining of key performance indicators

This thesis will utilize many of these features in order to model and compare passenger cars with and without a catalytic converter.

2.1 Assessment Methodologies

Within SimaPro, two analysis methodologies will be used: Eco-indicator 99 (hierarchist) and Cumulative Energy Demand. Eco-indicator 99 is a commonly used European model with a damage-oriented approach [27]. Eco-indicator 99 assesses the type of damage caused by various impact categories. The damage points are split up into three categories: Damage to Human Health, Damage to Ecosystem Quality, and Damage to Resources. Damage to Human Health is the number of years life lost and the number of years lived disabled. The combination of these two numbers is also known as Disability Adjusted Life Years (DALYs). Damage to Ecosystem

Quality is the loss of species over a certain time, in a certain area. Damage to Resources is the surplus energy required for future extractions of minerals and fossil fuels [27]. The hierarchist perspective of Eco-indicator 99 is used in this analysis. This version is moderate, assuming no extremes. The assumptions of this version include:

- Long-term time perspective
- Damages are avoidable by good management
- Fossil fuels are not substituted easily
- Age is not a factor in determining the Damage to Human Health (or DALYs)

The hierarchist perspective is the default method of Eco-indicator 99. In general, the assumptions made in this perspective are scientifically and politically accepted [27].

Cumulative Energy Demand is a single issue analysis methodology that combines all of the energy used throughout the life cycle of a product. Single issue means that the analysis only evaluates one subject, such as energy in this case. Cumulative Energy Demand divides energy resources into five impact categories [27]:

1. Non-renewable, fossil
2. Non-renewable, nuclear
3. Renewable, biomass
4. Renewable, wind, solar, geothermal
5. Renewable, water

In order to assess the relative contribution to the overall environmental impact based on assumptions, such as the precious metal used for the catalyst, sensitivity analysis will be used. This technique tests the original assumption by changing it to another possibility and recalculating the entire LCA. Sensitivity analysis determines how large of an effect a change to an input can have on the output [27]. The sensitivity analysis tests will analyze the emissions required during extraction and/or manufacture. This method will not assess the monetary cost of a material or product.

2.2 Materials

Figure 2.1 below is a picture of a disassembled sample catalytic converter from a typical passenger car under investigation in this LCA.

Figure 2.1: Cut-apart catalytic converter. (Photo by author, 2012).

The ceramic substrates are the three pieces at the top of the picture while the stainless steel casing is the four pieces at the bottom of the picture. Unlike many catalytic converters, this sample has two smaller reduction catalysts instead one large one, like the oxidation catalyst. The flow of pollutants goes from left to right; this can be seen by how much dirtier the reduction catalysts are versus the oxidation catalyst. Table 2.1 gives the weighed masses of the major components seen in Figure 2.1.

Table 2.1: Materials weighed from sample catalytic converter

Component	Mass (grams)
Ceramic substrates	832.3
Stainless steel casing	3865

As explained in the introduction, there are many materials that are necessary for the creation of a catalytic converter. There are also auxiliary materials, such as cardboard and plastic, used for the transportation of parts.

The exact mass of the ceramic substrate is dependent on the manufacturer, car model and engine. The total weight of the test ceramic substrates is 832.3 grams. Using the following weight percentages in Table 2.2, found from *Thermal Expansion of Extruded Cordierite Ceramics* by Lachman, Bagley, & Lewis, the amount of each material was found, and entered into the SimaPro model.

Table 2.2: Extruded ceramic cordierite batch composition [Lachman, I., Bagley, R., & Lewis, R. (1981). Thermal expansion of extruded cordierite ceramics. *Ceramic Bulletin*, *60*(2), 202-205.]. (Used under fair use, 2012).

Raw Material	Amount in composition (wt%)
Kaolin, $Al_2(Si_2O_5)(OH)_4$	21.74
Talc, raw, $Mg_3(Si_2O_5)_2(OH)_2$	39.24
Alumina, Al_2O_3	11.23
Aluminum hydroxide, $Al(OH)_3$	17.80
Silica, SiO_2	9.99
Totals	100.0

These raw materials will form into cordierite after processing. Equation 2.1 below provides the transformation of raw materials into cordierite

$$Al_2(Si_2O_5)(OH)_4 + Mg_3(Si_2O_5)_2(OH)_2 + Al_2O_3 + Al(OH)_3 + SiO_2 \longrightarrow \text{Cordierite} + \text{Water} \uparrow \quad (2.1)$$

As seen from this equation, cordierite is a combination of alumina (Al_2O_3), magnesia (MgO), and silica (SiO_2); the water is dried out during multiple processes. The energy for the water is accounted for in the materials in the SimaPro model. For ease of calculation, it is assumed that there is a 100 gram sample. The results will be scaled up to correlate to the actual data. The balanced form of Equation 2.1 for a 100 gram sample can be seen in Equation 2.2 below. The calculations and work for these numbers can be seen in Appendix A.1 on page 61.

$$0.08\ Al_2(Si_2O_5)(OH)_4 + 0.10\ Mg_3(Si_2O_5)_2(OH)_2 + 0.11\ Al_2O_3 + 0.23\ Al(OH)_3 + 0.17\ SiO_2 \rightarrow$$
$$0.31\ Al_2O_3 + 0.75\ SiO_2 + 0.31\ MgO + 0.61\ H_2O \quad (2.2)$$

The output moles of each compound can be converted into output masses by multiplying these moles by the molecular weight of each compound. This will determine the masses of cordierite and water for the 100 gram sample. The mass of cordierite for the sample in the experiment was determined to be 832.3 grams. The masses of alumina, magnesia, silica and water can be found by scaling the 100 gram sample to the experimental data. Once the output data is known for the experimental data, the input masses can be determined. The work all of these numbers can also be seen in Appendix A.1 on page 61. Table 2.3 below gives the input and output masses for the experimental data. The input and output mass totals are slightly different due to rounding throughout the calculation. The input masses for kaolin, talc, alumina, aluminum hydroxide and silica are entered into SimaPro.

Table 2.3: Masses for all inputs and outputs for the cordierite substrate

	Material	**Mass (grams)**
Inputs	Kaolin	194
	Talc	357
	Alumina	102
	Aluminum Hydroxide	172
	Silica	96
Outputs	Alumina	300
	Silica	416
	Magnesia	117
	Water	103

The output masses can be used to determine the placement of this composition on a ternary phase diagram. Figure 2.2 below gives the ternary system for MgO- Al_2O_3- SiO_2 [28]. In this system, there is a cordierite phase section. In this phase there are varying compositions of cordierite that are stable. The composition of cordierite used in this analysis, see Table 2.2 for the batch mixture, can be pinpointed on this system. The black 'o' indicates the location of this composition of cordierite. Found by using the output weight percent of silica, magnesia and alumina, this location is the placement of 2 Al_2O_3 – 2 MgO – 5 SiO_2. There is a total of approximately 833 grams of cordierite in the analysis sample. From Table 2.3, the cordierite composition is about 50 weight percent silica; therefore, the placement is determined by going five arrow notches down from the silica peak. The composition is about 36 weight percent alumina; in the same manner, a line is drawn six and a half arrow notches away from the alumina peak. The composition is about 14 weight percent magnesia; the line placement is about nine and a half arrow notches away from the magnesia peak. Three lines can be drawn from these placements, and where they intersect the cordierite composition can be seen.

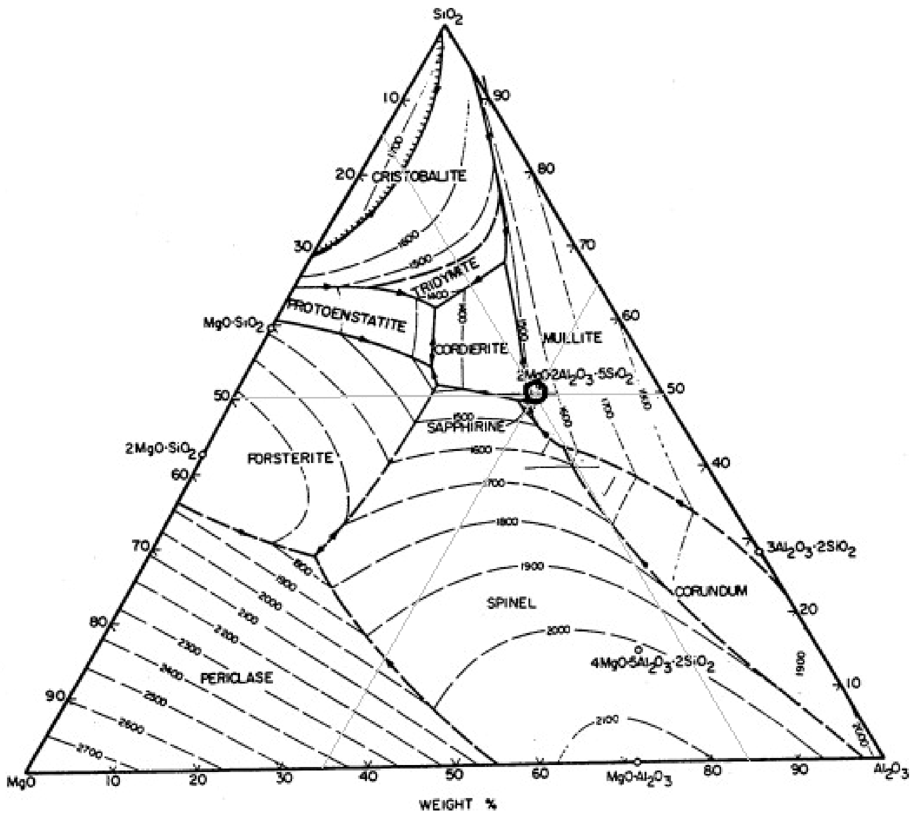

Figure 2.2: The ternary system MgO-Al_2O_3-SiO_2 (in weight percent) [Benito, J.M., Turrillas, X., Cuello, G.J., De Aza, A.H., De Aza, S., Rodríguez, M.A. (2012). Cordierite synthesis. A time-resolved neutron diffraction study. *Journal of the European Ceramic Society*, *32*(2), 371-379, Retrieved from http://www.sciencedirect.com/science/article/pii/S0955221911004766]. (Used under fair use, 2012)

The catalyst is applied to the ceramic substrate in two steps. First, a washcoat is applied to the bare monolith. This coating was found to weigh approximately 278.5 grams. This calculation can be seen in Appendix A.2 on page 68. The washcoat is made by mixing 100 parts by weight of fine-grained alumina with 4 parts by weight of one or more fine-grained powders of a rare earth metal oxide, such as cerium oxide [25]. This mixture is then suspended in 250 parts by weight of water.

Second, a metal catalyst coating is applied to the washcoated ceramic substrate. A composite powder of 5 parts platinum, 1 part rhodium, and 60 parts lanthanum oxide is mixed together. In a similar manner as the washcoat, the ceramic substrate is dipped into a mixture of 1 part composite powder and 50 parts water. The substrate is dipped until 1.5 grams of noble metals have been applied on the substrate per liter of the volume of the substrate [25]. The geometric volume of the substrates is estimated to be 2.2 liters; this volume is found by measuring the geometry of the substrate and calculating the volume. This equates to a total of 3.3 grams of noble metal. The components are placed into a canister made of type 409 stainless steel. The canister used for the study weighed approximately 3865 grams.

Auxiliary materials are those required during the production of the product, but are not an actual material in the product. The packaging necessary for shipping and transporting a catalytic converter from manufacturers are auxiliary materials. When the ceramic monolith leaves the first manufacturer, six to twenty-four are placed in a cardboard box with low density polyethylene (LDPE) plastic supporting the tops and bottoms. The same kind of packaging is used once the ceramic monolith has been coated and leaves the second manufacturer. After the third manufacturer, where the stainless steel housing is fitted, a single converter is placed in a plastic bag in a cardboard box, and filled with packing paper. The packaging materials are assumed to be small since in the first two steps, multiple substrates were in each box. The plastic and paper filler are left out of the analysis because there is so little used per converter. Using a packaging calculator, the weight of a box 24 inches in length, 12 inches in width and 12 inches in height, is 628.2 grams [29]. Assuming twelve ceramic substrates are in each box, and two are used per converter, the combined weight of the boxes for the first and second manufacturer is 209.4 grams. The third manufacturer uses an entire box, 628.2 grams, for one converter. The material required for all three manufacturers is 837.6 grams.

Table 2.4 below gives the major materials necessary for the creation of a catalytic converter. The table is broken up into five parts, the substrate, the catalyst coating (washcoat), the catalyst coating (metal), the canister, and the packaging. The masses are weighed and estimated from the sample catalytic converter. The last column in the table provides details on the material processes selected in SimaPro. The specific name of the material is given and the database where the information came from is in the parentheses. These processes are essentially LCA studies of the inputs and outputs required to extract and manufacture these materials which are then used as inputs in this catalytic converter model.

Table 2.4: Materials used in a catalytic converter

Catalytic converter component	**Material**	**Mass (grams)**	**SimaPro selection**
Ceramic substrate	Kaolin	194	Kaolin, at plant/RER U (from Ecoinvent)
	Talc, raw	357	Talc, in ground (from Raw materials)
	Alumina	102	Alumina, at plant/US (from U.S. LCI Database)
	Aluminum hydroxide	172	Aluminum hydroxide, at plant/RER U (from Ecoinvent)
	Silica	96	Silica sand, at plant/DE U (from Ecoinvent)
Catalyst coating (washcoat)	Alumina	268	Alumina, at plant/US (from U.S. LCI Database)
	Rare earth oxide	10.7	Cerium oxide, at plant S (from Ecoinvent)
Catalyst coating (metal)	Lanthanum oxide	3.02	Lanthanum oxide, at plant/CN S (from Ecoinvent)
	Platinum	0.25	Platinum, primary, at refinery/RU S (from Ecoinvent)
	Rhodium	0.050	Rhodium, primary at refinery/RU S (from Ecoinvent)
Canister	Stainless steel (type 409)	3865	Stainless steel hot rolled coil, grade 304 RER S (from ELCD 2.0)
Packaging	Cardboard	837.6	Corrugated board boxes, technology mix (from ELCD 2.0)

2.3 Processing

Various processing steps are necessary to convert the raw materials into the catalytic converter. Figure 1.2 provides the process flow diagram. The electricity used for processing of the ceramic is assumed to be from southwest Virginia. The electricity mix from American Electric Power for southwest Virginia was used in SimaPro can be seen in Table 2.5 below [30].

Table 2.5: Electricity fuel mix for southwest Virginia per kWh [AEP's average fuel mix of electricity provided to Virginia customers. In (2010). *2010 Environmental Information.*]. (Used under fair use, 2012).

Electricity type	**Amount (kWh)**
Electricity, hard coal, at power plant/US U	0.842
Electricity, nuclear, at power plant/US U	0.12
Electricity, natural gas, at power plant/US U	0.022
Electricity, hydropower, at power plant/ SE U	0.005
Electricity, at wind power plant/RER U	0.011

The first processing step is the creation of the ceramic monolith structure. This process is just one of the various methods used for the ceramic substrates. Different manufacturers may use different methods, including various techniques of shaping, drying and firing. The ceramic raw materials are received at plant and are measured and mixed together. Next, the raw materials, including organic binders, are extruded into long continuous logs. The ceramic is wet cut into smaller pieces. The wet ceramic is then microwave dried to remove moisture. The dried ceramic is green cut into the desired size for the catalytic converter. Using a progressive kiln or tunnel kiln, the ceramic pieces are fired. During firing, the organic binders and water are released from the product and into the air without collection; the organic binders are not included in this analysis as mentioned previously. After firing, the ceramic piece goes through inspection and packaging. This structure is then transported to the second facility for the addition of the metal catalyst. Table 2.6 below gives energies for various processing methods for magnesia brick refractories [31]. Due to a lack of published data on cordierite processing energies, these energies will be used in the analysis. To account for variability between the energies for cordierite compared to magnesia brick, the drying and firing energies will be tested with sensitivity analysis. One test will take 50% of these energies to provide analysis results for the event that the cordierite processing energy far less than that for magnesia brick. The second test will take 75% of the drying and firing energies to provide analysis results for the event that the cordierite processing energy is somewhat smaller that for magnesia brick.

Table 2.6: Energy consumption data for the processing of magnesia refractory bricks [*Reference document on best available techniques in the ceramic manufacturing industry*. (2007). Retrieved from http://eippcb.jrc.es/reference/BREF/cer_bref_0807.pdf]. (Used under fair use, 2012).

Process	**MJ/kg**
Preparation, screening	0.35-0.50
Weighing, dosing, mixing	0.045-0.070
Shaping	0.13-0.20
Conventional drying and firing	3.0-6.3
Subsequent treatment, packaging	0.08

The averages of these ranges were used in the SimaPro model for each process. Cutting and extrusion both fall under the shaping, and there are two forms of cutting; therefore, this energy is multiplied times three. The drying, firing process uses the average value, but is modified based on the fact that it is a combined range using conventional methods for drying and firing. The modifications will divide the energy range into microwave drying and conventional drying energies. The microwave energy for refractories can be found in Table 2.7 below [32]. This table provides the drying and firing energies for various ceramics over a year. This table will be used along with Table 2.6 to modify the drying and firing energy.

Table 2.7: Microwave energy savings potential in ceramics manufacturing [Sheppard, L. (1988). Manufacturing ceramics with microwaves: the potential for economical production. *Ceramic Bulletin*, *67*(10), 1656-1660]. (Used under fair use, 2012).

	Conventional drying (x 10^6 kW·h/yr)	**Microwave drying** (x 10^6 kW·h/yr)	**Conventional firing** (x 10^6 kW·h/yr)	**Microwave firing** (x 10^6 kW·h/yr)	**Total energy savings** (x 10^6 kW·h/yr)
Brick and tile	56.10	28.05	198.90	19.90	207.06
Electrical porcelain	3.52	1.76	12.48	1.25	12.99
Glazes	16.63	8.30	58.97	5.89	61.37
Pottery	1.96	0.98	6.94	0.69	7.23
Refractories	10.87	5.40	38.53	3.85	40.08
Sanitary ware	25.04	12.52	88.76	8.88	92.40
Advanced ceramics	1.30	0.65	4.60	0.46	4.79
Total (x 10^6 kW·h/yr)	115.42	57.66	409.18	40.92	425.92
(x 10^6 PJ/yr)	0.42	0.21	1.47	0.15	1.50

The range, from Table 2.6, given for conventional drying and firing is 3.0 – 6.3 MJ/kg. Looking at Table 2.7, the energies for conventional drying and firing of refractories can be used to determine a total energy, and then the percentage due to conventional drying. Equation 2.3

provides the total energy for these processes. Equation 2.4 gives the conventional drying as a percentage of the total energy.

Total conventional energy for a refractory = Refractory conventional drying energy + Refractory conventional firing energy

$$Total\ conventional\ energy\ for\ a\ refractory = 10.87\ \text{x}\ 10^6\ \text{kW} \cdot \text{h/yr} + 38.53\ \text{x}\ 10^6\ \text{kW} \cdot \text{h/y} = 49\text{x}\ 10^6\ \text{kW} \cdot \text{h/yr} \quad (2.3)$$

$$Conventional\ Drying\ Percentage = \frac{10.87\text{x}\ 10^6\ \text{kW·h/yr}}{49.4\text{x}\ 10^6\ \text{kW·h/yr}} \times 100\% = 22.00\% \quad (2.4)$$

This percentage can be applied to the given range for drying and firing in Table 2.6 to estimate how much energy is due to the drying. Applying 22% to the drying, firing range of 3.0 – 6.3 MJ/kg yields a drying range of 0.66 – 1.39 MJ/kg. The remaining 2.34 – 4.91 MJ/kg is the range for conventional firing of a refractory.

Referencing Table 2.7 again, the conventional drying and microwave drying energies for a refractory can be compared. Equation 2.5 gives the microwave drying energy as a percentage of conventional drying energy.

Microwave drying percentage for a refractory = Refractory microwave drying energy / Refractory conventional drying energy

$$Microwave\ Drying\ Percentage = \frac{5.40}{10.87} \times 100\% = 49.7\% \quad (2.5)$$

This percentage can be applied to the conventional drying range, 0.66 – 1.39 MJ/kg, to find the microwave drying range. This range is found to be 0.328 – 0.689 MJ/kg. Since this range is characteristic of refractories, and not specifically cordierite, the average value, 0.508 MJ/kg, is used in the analysis.

Table 2.8 below provides the energies per weight basis for all of the ceramic processing methods. As stated above, the average value for each range is used in the SimaPro model. The last two columns provide the energies used in the two sensitivity analysis tests. Only the drying and firing energies will be tested since the screening, mixing, shaping and packaging energies are not expected to vary between the two materials.

Table 2.8: Energy data entered into SimaPro for the processing phase [31, 32]

Process	**MJ/kg**	**50% of the drying and firing energy MJ/kg**	**75% of the drying and firing energy MJ/kg**
Preparation, screening	0.425	0.425	0.425
Weighing, dosing, mixing	0.058	0.058	0.058
Shaping	0.165	0.165	0.165
Microwave Drying	0.508	0.254	0.381
Firing	3.627	1.814	2.720
Subsequent treatment, packaging	0.08	0.08	0.08
Total	4.863	2.796	3.829

When the ceramic structure arrives at the second facility, it is coated with a washcoat and metal catalyst. The alumina, rare earth metal oxide, and water are mixed, and the ceramic structure is dipped into this mixture and subsequently sintered at 500°C in contact with air [25]. In order to create the composite powder of noble metals, chloroplatnic acid (H_2PtCl_6), rhodium nitrate ($Rh(NO_3)_3$), and lanthanum nitrate ($La(NO_3)_3$) are sprayed into a reactor with an atmosphere containing oxygen at approximately 950°C. The resulting composite powder is again mixed with water. The washcoated ceramic structure is dipped, dried and sintered at 500°C in contact with air. As explained above, this process of dipping, drying and sintering the catalyst mix is repeated until a desired amount of noble metal is reached [25]. Once the catalyst coated ceramic passes inspection, it is packaged and shipped to the third and final manufacturing facility.

The final processing necessary for a catalytic converter is the stainless steel housing. Made out of type 409 ferritic stainless steel, the canister has a tube-like body with one open end and one end tapered to a reduced diameter to allow for a connection to the exhaust system pipe [33]. The housing shells are processed by deep drawing, in which the usual conical ends are modified to provide the open and tapered ends. SimaPro has a deep drawing process built into the software that is used in the model for this process step. Various pressures for deep drawing were available, but a high pressure of 38000 kN was chosen. This decision was based on the fact that ferritic stainless steels work-harden faster than carbon steels, and therefore need higher pressures to form [34].   The process selected in SimaPro is, “deep drawing, steel, 38000 kN press, automode operation/kg/RER”. The data for the process is published in *Life Cycle Inventories of Metal Processing and Compressed Air Supply* in 2007 by R. Steine and R. Frischknecht. The shells are joined together, generally by welding [33]. Once the catalytic converter is fully constructed, it is packaged and shipped to the customer.

2.4 Usage

Once the catalytic converter is installed in a vehicle, it begins its use phase. It is in this phase that the product makes a positive environmental contribution. In order to examine the benefits of the catalytic converter in use, a comparison of a vehicle with and without the catalytic converter will be used. The emissions for both of these models can be seen in Table 2.9 below. This data is for an average passenger car taken from the second edition of *Air Pollution: Measurement, Modeling and Mitigation* by Jeremy Colls [35]. The data has been converted from grams per kilometer to grams per mile.

Table 2.9: Average passenger car emissions with and without a catalytic converter [Colls, J. (2002). *Air pollution: measurement, modelling, and mitigation*. (Second ed., pp. 127-137). New York, NY: Spon Press.]. (Used under fair use, 2012).

	Carbon monoxide (g/mi)	Hydrocarbons (g/mi)	Nitrogen oxides (g/mi)
Gasoline car without a catalytic converter	43.5	4.51	2.74
Gasoline car with a catalytic converter	3.22	0.322	0.644

The numerical difference between the car without a catalytic converter and the car with a catalytic converter is the amount of emissions converted to less harmful pollutants. Both carbon monoxide and hydrocarbons are converted to carbon dioxide by the catalytic converter. Table 2.10 provides the converted emissions.

Table 2.10: Converted emissions for an average passenger car [Colls, J. (2002). *Air pollution: measurement, modelling, and mitigation*. (Second ed., pp. 127-137). New York, NY: Spon Press.]. (Used under fair use, 2012).

	Carbon monoxide (g/mi)	Hydrocarbons (g/mi)	Nitrogen oxides (g/mi)
Converted emission	40.2	4.18	2.09

Equations 2.6 and 2.7 provide the conversion factors to carbon dioxide. The masses of CO_2 and CO are based on the balanced equation seen in Equation 1.3. Since there are various forms of hydrocarbons, the common form of benzene is used in this conversion [19]. The masses of HC and CO_2 are based on the balanced equation seen in Equation 1.5.

$$CO\ converted\ \times \frac{mole \times molecular\ weight\ of\ CO_2}{mole \times molecular\ weight\ of\ CO} = 40.2 \frac{g}{mi}\ CO \times \frac{2 \times 44.009\ g\ CO_2}{2 \times 28.01\ g\ CO} = \ 63.2 \frac{g}{mi}\ CO_2 \qquad (2.6)$$

$$C_6H_6\ converted \times \frac{mole \times molecular\ weight\ of\ CO_2}{mole \times molecular\ weight\ of\ C_6H_6} = 4.18 \frac{g}{mi}\ C_6H_6 \times \frac{12 \times 44.009\ g\ CO_2}{2 \times 78.114\ g\ C_6H_6} = 3.38 \frac{g}{mi}\ CO_2 \qquad (2.7)$$

According to the EPA, the amount of carbon dioxide in a gallon of gasoline can be found by Equation 2.8 below [36]. The average heat content in a gallon of gasoline is 0.125 mmbtu/gallon; the average carbon dioxide emissions per heat content of gasoline is 71.35 kg CO_2/mmbtu.

$$0.125 \frac{mmbtu}{gallon} \times 71.35\ \frac{kg\ CO_2}{mmbtu} = 8.92\ \frac{kg\ CO_2}{gallon} \qquad (2.8)$$

From this equation, it is determined that gasoline emits approximately 8.92 kilograms of carbon dioxide per gallon of gasoline [36]. The car modeled in this study has a combined city and highway fuel economy of 24 miles per gallon [37]. Table 2.11 below provides all of the vehicle emissions for one functional unit (80,000 miles). The work for these numbers can be found in Appendix A.3 on page 69.

Table 2.11: Vehicle emissions for one functional unit

	Carbon monoxide (kg)	Hydrocarbons (kg)	Nitrogen oxides (kg)	Carbon dioxide (kg)
Car without a catalytic converter	3480	360.8	219.2	29730
Car with a catalytic converter	257.6	25.76	51.52	35920

When comparing the car without the converter to the car with the converter, CO, HC and NO_x emissions are all decreased. The carbon dioxide emissions, however, increase when comparing a car without a converter to a car with a converter. The same amount of gasoline is used in each car, giving both cars 29730 kg of carbon dioxide; however, the car with a catalytic converter also has 6190 kilograms of carbon monoxide and hydrocarbons converted into carbon dioxide.

2.5 Disposal

The disposal phase, that is the end of life disposition for the catalytic converter, will not be modeled in SimaPro. This is because an emission comparison is the primary objective in this life cycle analysis; while energy consumption is considered, it is not the major goal of the analysis. The disposal phase is also not expected to add any significant emissions. Since these materials do not break down quickly into hazardous materials at the landfill, the disposal impacts are mainly due to the transportation of used parts to the landfill. This transportation and associated emissions are very small compared to the functional unit of 80,000 miles. Also, the energies associated with the reclamation process of precious metals are not commonly available. Just because it is not modeled does not mean it is not important. Currently about 50% of catalytic converters are recycled [38]. When a catalytic converter is recycled, the stainless steel canister and precious metals are recycled, and the remaining ceramic is landfilled. In order to recycle type 409 stainless steel, energy is required. Table 2.12 provides the energy required to produce virgin steel versus recycle the steel. Embodied energy is the total of all energy required for a product throughout its entire product lifecycle [39]. More than three times the energy is required to process virgin stainless steel instead of recycling it.

Table 2.12: Processing versus recycling energies for type 409 stainless steel [Stainless steel, ferritic, AISI 409, wrought, annealed. In (2011). *CES EduPack 2011*]. (Used under fair use, 2012).

Type of Energy	**Energy (MJ/kg)**
Embodied energy, primary production	77.2 – 85.3
Embodied energy, recycling	21.6 – 23.9
Energy savings	55.6 – 61.4

Catalytic converters utilize about one third of the world's supply of platinum, and 87% of the world's supply of rhodium [40]. The precious metals are valuable when recycled because of their resource rarity and monetary value. In the same manner as stainless steel, when precious metals are recycled, energy is required. Table 2.13 below provides the energy required to produce platinum and rhodium versus recycle the metals [41, 42].

Table 2.13: Processing versus recycling energies for platinum and rhodium [Platinum, commercial purity, P04995, annealed. In (2011). *CES EduPack 2011*, and Platinum-rhodium alloy, annealed. In (2011). *CES EduPack 2011*]. (Used under fair use, 2012).

Precious Metal	**Type of Energy**	**Energy (MJ/kg)**
Platinum	Embodied energy, primary production	$1.14 \cdot 10^5$
	Embodied energy, recycling	$1.08 \cdot 10^3 - 1.2 \cdot 10^3$
	Energy savings	$1.13 \cdot 10^5 - 1.13 \cdot 10^5$
Rhodium	Embodied energy, primary production	$1.22 \cdot 10^5 - 1.35 \cdot 10^5$
	Embodied energy, recycling	$2.44 \cdot 10^3 - 2.7 \cdot 10^3$
	Energy savings	$1.20 \cdot 10^5 - 1.32 \cdot 10^5$

Tremendous amounts of energy can be saved when these precious metals are recycled compared to virgin production. While the energy savings are important, the available metal for reuse is the primary desire. During the reclamation of the precious metals, 80 to 94 percent of platinum can be recovered, while 65 to 90 percent of rhodium can be recovered [43]. Comparing Tables 2.12 and 2.13, it can be seen how much more energy is required to produce platinum and rhodium over stainless steel. More energy is required to extract and process these rare metals because it is a time and energy intensive process.

According to the United States Bureau of Transit Statistics for 2009, there are over 254 million registered passenger vehicles in the United States [44]. If only half of these will be recycled at some point in time, then approximately 127 million catalytic converters will be landfilled. This number is also assuming only one catalytic converter is used per car, when in reality this number would be even greater. The average landfill is 116 acres [45]. The size of the catalytic converter is less than two square feet, and there are 43,560 square feet in one acre. While there is some land use, the amount of volumetric space that would be required for this many components is not significant.

3.0 Results of Analysis

Once all of the data was entered into SimaPro, two models, Car with Catalytic Converter and Car without Catalytic Converter, were compared. In this comparison, the life cycle inventory was used to determine the total of the key emissions (carbon monoxide, hydrocarbons, nitrogen oxides and carbon dioxide). The environmental impact and total energy usage were quantified as well.

3.1 Comparison of Key Emissions

Table 3.1 below gives the inventory results for total carbon monoxide. There is a row specifically for the emissions occurring during the use phase, and a row for the emissions during extraction and processing (labeled manufacture). How the emission is input or output can be found in the column "Compartment". The full emission tables for all of the key emissions can be found in Appendix B on page 73.

Table 3.1: Total emissions for carbon monoxide

Emission	Compartment	Unit	Car with Catalytic Converter	Car without Catalytic Converter
Carbon monoxide, usage	Air	kg	258	3480
Carbon monoxide, manufacture	Air	kg	0.192	-
Total		kg	258	3480

Table 3.2 below gives the total emissions for hydrocarbons. Again, one row is the hydrocarbons emitted during usage, and the second row is the hydrocarbons emitted due to the creation of a catalytic converter.

Table 3.2: Total emissions for hydrocarbons

Emission	**Compartment**	**Unit**	**Car with Catalytic Converter**	**Car without Catalytic Converter**
Hydrocarbons, usage	Air	kg	25.8	360
Hydrocarbons, manufacture	Air and Water	kg	0.000158	-
Total		kg	25.8	360

Table 3.3 below gives the total emissions for nitrogen oxides. The NO_x emitted during use is in one row while the extraction and processing NO_x emissions are in a separate row.

Table 3.3: Total emissions for nitrogen oxides

Emission	**Compartment**	**Unit**	**Car with Catalytic Converter**	**Car without Catalytic Converter**
Nitrogen oxide (NO_x) usage	Air	kg	51.5	219
Nitrogen oxide (NO_x) manufacturing	Air	kg	0.1	-
Total		kg	51.6	219

Table 3.4 below gives the total emissions for carbon dioxide. The emissions due to usage and manufacture are again split into two separate rows, with a total CO_2 emission for a car with and without a catalytic converter.

Table 3.4: Total emissions for carbon dioxide

Emission	**Compartment**	**Unit**	**Car with Catalytic Converter**	**Car without Catalytic Converter**
Carbon dioxide, Usage	Air	kg	35920	29730
Carbon dioxide, manufacture	Air and Raw	kg	23.6	-
Total		kg	35940	29730

Table 3.5 below gives the total emissions for all key emissions. The last column, "emission differences" gives the increase or decrease of emissions based on a car without a catalytic converter compared to a car with a catalytic converter.

Table 3.5: Total emissions for all key emissions

Emission	**Unit**	**Car without Catalytic Converter**	**Car with Catalytic Converter**	**Emission Differences**
Carbon monoxide	kg	480	258	– 222
Hydrocarbons	kg	360	25.8	– 334
Nitrogen oxides	kg	219	51.6	– 167
Carbon dioxide	kg	29730	35940	+ 6210

3.1.1 Sensitivity Analysis

As previously discussed, sensitivity analysis was used in order to test the effect that assumptions may have on the outcome of the life cycle. Five assumptions were tested:

- Platinum is solely used as the oxidation catalyst.
- Alumina is solely used as the bulk of the washcoat.
- The ceramic processing energies are the averages for the magnesia brick.
- Microwave drying is used.
- Conventional firing is used.

The assumption that solely platinum was used as the oxidation catalyst was tested by changing the assumption to include palladium as the oxidation catalyst. Platinum was initially used as the oxidation catalyst, but was eventually switched to palladium because it is cheaper [40]. In 2000, palladium prices peaked and car makers switched back to platinum, but they are now going back to platinum. Since cars currently on the road can have platinum or palladium, a sensitivity tests was run. In this test, 100% palladium was used for the oxidation catalyst. Table 3.6 below gives the total emissions for the initial scenario of 100% platinum and the difference in emissions for the sensitivity analysis test.

Table 3.6: Sensitivity analysis of platinum

Emission	**Unit**	**Emissions for a car with 100% platinum**	**Emission differences for a car with 100% palladium**
Carbon monoxide	kg	258	- 0.0046
Hydrocarbons	kg	25.8	- 0.0000041
Nitrogen oxides	kg	51.6	+ 0
Carbon dioxide	kg	35920	- 1.11

The assumption that all alumina was used as the bulk of the washcoat was tested by changing the assumption to include silica. The first sensitivity test replaces all alumina with all silica. The second sensitivity test uses a composite of 50% alumina and 50% silica. The results of the sensitivity analysis can be seen in Table 3.7 below.

Table 3.7 Sensitivity analysis of alumina

Emission	**Unit**	**Emissions for a car with 100% alumina**	**Emission differences for a car with 100% silica**	**Emission differences for a car with 50% alumina and 50% silica**
Carbon monoxide	kg	258	- 0.001	+ 0.020
Hydrocarbons	kg	25.8	+ 0	+ 0.000016
Nitrogen oxides	kg	51.6	+ 0	+ 0
Carbon dioxide	kg	35920	- 0.35	+ 2.54

The assumption that the cordierite processing energies are the average of the magnesia brick processing energies (total of 4.863 MJ/kg) was tested by changing the assumption to 50% and 75% of the drying and firing energies. The first sensitivity test replaces the average energy values for drying and firing with half of the average energy values (total of 2.796 MJ/kg). The second sensitivity test uses three-quarters of the average energy values for drying and firing (total of 3.829 MJ/kg). The results of the sensitivity analysis can be seen in Table 3.8 below.

Table 3.8 Sensitivity analysis of cordierite processing energy

Emission	Unit	Emissions for a car with average energy (4.863 MJ/kg)	Emission differences for a car with 50% energy (2.796 MJ/kg)	Emission differences for a car with 75% energy (3.829 MJ/kg)
Carbon monoxide	kg	258	- 0.0002	- 0.0009
Hydrocarbons	kg	25.8	- 0.000022	- 0.000011
Nitrogen oxides	kg	51.6	+ 0	+ 0
Carbon dioxide	kg	35920	- 0.29	- 0.15

Sensitivity analysis is conducted on the assumption that microwaves are used during the drying process of the ceramic substrates. The assumption is changed so that conventional drying is used instead of microwave drying. The energy used for conventional drying 1.023 MJ/kg. This is the average of the energy range determined by Equations 2.3 and 2.4. The results of the analysis can be found in Table 3.9 below.

Table 3.9 Sensitivity analysis of microwave drying

Emission	Unit	Emissions for a car with microwave drying	Emission differences for a car with conventional drying
Carbon monoxide	Kg	258	+ 0.0011
Hydrocarbons	Kg	25.8	- 0.00000051
Nitrogen oxides	Kg	51.6	+ 0
Carbon dioxide	Kg	35920	+ 0.23

Sensitivity analysis is also conducted on the assumption that conventional furnaces are used during the firing process of the ceramic substrates. The assumption is changed so that microwave firing is used instead of conventional firing. The energy used for microwave firing is

0.7248 MJ/kg. This is the average of the energy range determined by Equations A.11, A.12 and A.13 Appendix A.4 on page 71. The results of the analysis can be found in Table 3.10 below.

Table 3.10 Sensitivity analysis of conventional firing

Emission	**Unit**	**Emissions for a car with conventional firing**	**Emission differences for a car with microwave firing**
Carbon monoxide	kg	258	- 0.0008
Hydrocarbons	kg	25.8	- 0.000043
Nitrogen oxides	kg	51.6	+ 0
Carbon dioxide	kg	35920	- 0.02

3.2 Eco-indicator 99 (H)

Using Eco-indicator 99 (H), Figure 3.1 below compares the damages for human health, ecosystem quality and resources in terms of percentage. Each of the three damage categories compares the damages for a car with and without a catalytic converter, setting the higher value at 100% for ease of comparison. These values are normalized by the total amount of damage in Europe assigned to an average citizen (per capita).

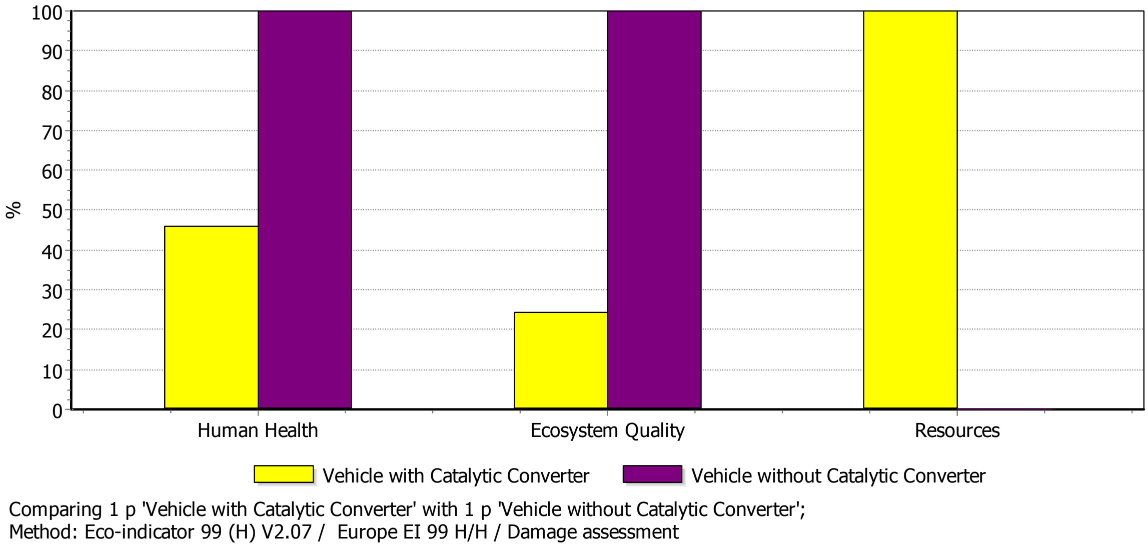

Figure 3.1 Eco-indicator 99 damage assessment chart for a car with and without a catalytic converter

Table 3.11 below corresponds to the figure above, providing numbers to relate to the percentages. For example, 0.0125 DALY is about 46% of 0.0273 DALY; therefore, the human health bar for a car without a catalytic converter is 100%, and the bar for a car with a catalytic converter is approximately 46%. In this table, the unit PDF · m^2 · yr is the percentage of loss species, multiplied by the area, multiplied by a time increment [27]. The unit MJ surplus is the surplus energy needed for future extractions of minerals and fossil fuels.

Table 3.11 Eco-indicator 99 numerical damage assessment for a car with and without a catalytic converter

Damage category	**Unit**	**Car with catalytic converter**	**Car without catalytic converter**
Human Health	DALY	0.0125	0.0273
Ecosystem Quality	PDF · m^2 · yr	304	1250
Resources	MJ surplus	19.6	0

Tables 3.12, 3.13 and 3.14 below provide the top three contributors to the damages seen above for a car with a catalytic converter. In the case of a car without a catalytic converter, all of the environmental points come from the process, “emissions during use without a converter”.

Table 3.12: Top three contributors to the damage to human health

Number	**Process**	**DALY**
1	Emissions during use with converter	0.0122
2	Platinum, primary, at refinery	0.000182
3	Rhodium, primary, at refinery	0.0000796

Table 3.13: Top three contributors to the damage to ecosystem quality

Number	**Process**	**PDF $\cdot$ m^2 $\cdot$ yr**
1	Emissions during use with converter	294
2	Platinum, primary, at refinery	4.41
3	Stainless steel	2.85

Table 3.14: Top three contributors to the damage to resources

Number	**Process**	**MJ surplus**
1	Stainless steel	6.86
2	Platinum, primary, at refinery	4.77
3	Rhodium, primary, at refinery	2.09

3.3 Cumulative Energy Demand

Using Cumulative Energy Demand, Table 3.15 provides the total energy required to create a single catalytic converter, including extraction and manufacturing. A car without a catalytic converter does not require excess energy to create the component, and therefore does not have any energy associated with it. The energy is divided into six impact categories; these categories are the various forms of energy used during extraction and manufacturing.

Table 3.15: Cumulative energy demand characterization of energy usage

Impact Category	Material (MJ)	Processing (MJ)	Usage (MJ)	Total (MJ)
Non-renewable, fossil	195	26.7	0	221.7
Non-renewable, nuclear	23.4	3.48	0	26.88
Non-renewable, biomass	0.00293	$1.77 \cdot 10^{-5}$	0	0.0029477
Renewable, biomass	1.08	0.441	0	1.512
Renewable, wind, solar, geothermal	7.12	0.0597	0	7.1797
Renewable, water	2.8	0.33	0	3.13
Total	229.4	31.01	0	260.4

4.0 Discussion of Analysis Results

The purpose of this life cycle analysis is to determine whether or not a catalytic converter is a positive environmental product; so the basic question is, is it? Overall, the catalytic converter can be seen as having both positive and negative environmental impacts. The carbon monoxide, hydrocarbons and nitrogen oxides are all significantly decreased with the use of a catalytic converter. On the other hand, resources and energy are utilized, and the carbon dioxide emissions are increased considerably. While the car with a catalytic converter uses more energy, resources and outputs more carbon dioxide, it still has a lower environmental impact compared to a car without a catalytic converter. Whether or not the prevented pollutants outweigh the resources used is dependent upon the subjective weighting of importance for each category by individuals, corporations or governments. The air pollutant reductions lead to better short term health effects in the current population while the carbon dioxide emissions warm the atmosphere and have more uncertain long term health and ecosystem effects.

4.1 Key emissions

The use of a catalytic converter decreases the carbon monoxide emission by 222 kg, per functional unit, which is 80,000 miles. Carbon monoxide can disrupt the flow of oxygen in the bloodstream, causing serious problems with the brain, heat and other vital organs. Since carbon monoxide can be extremely hazardous to human health, the more that can be prevented, the better. The EPA has determined standards for safe carbon monoxide exposure; any exposure beyond these limits can be toxic [46]. The standards are 9 parts per million (ppm) over an 8-hour time span or 35 ppm over a 1-hour time span. Across the United States, concentrations above these standards have declined nearly 70% since 1990 [46].

In addition to carbon monoxide from the use phase emissions, there are some small CO emissions from the rest of the process including energy use. In the model, the majority, or 88%, of the carbon monoxide produced is from the manufacture of stainless steel. Alumina extraction and processing and deep drawing are the next largest contributors. Overall, the carbon monoxide emissions created from extraction and processing are small compared to the use phase. This indicates that creating the catalytic converter does not contribute a substantial amount of carbon monoxide emissions.

Hydrocarbons are reduced by 334 kg per 80,000 miles. In large cities where there is greater population and vehicles, the prevention of hydrocarbons and smog is very important. Figure 4.1 below shows Los Angeles, California in 1970 versus present day [47, 48].

Figure 4.1: Los Angeles in 1970 versus present day [Kempler, S. NASA, (2011). *Amateur guide for air quality testing* . Retrieved from website: http://disc.sci.gsfc.nasa.gov/oceancolor/additional/science-focus/locus/amateur_guide_for_air_quality_000.shtml, and (n.d.). *Los angeles*. [Web Photo]. Retrieved from http://www.stratosjets.com/featured-jet-charter/Jet-Charter-Flights-in-Los-Angeles]. (Used under fair use, 2012).

In 1970, Los Angeles and other large cities across the nation were plagued with smog. Due to the introduction of the Clean Air Act of 1970, and catalytic converters, large formations of urban smog have greatly decreased [10]. This can be seen in the present day photo of the city.

Considering a car with a catalytic converter, the hydrocarbons produced from extraction and processing are negligible. The emissions are so small that they do not even show up in the total hydrocarbon emissions; the emissions during the use phase completely dominate the hydrocarbon total.

Nitrogen oxides (NO_x) are decreased by 167 kg, per functional unit, with the use of a catalytic converter. Decreasing the amount of NO_x polluted into the air also decreases the negative environmental and health effects. The effects that can be prevented include acid rain, smog, lung irritation and respiratory problems. The more NO_x converted to less harmful emissions, the smaller the potential for acid rain and ozone formation. Again, there are very little emissions of NO_x during the extraction and processing of creating a catalytic converter. The NO_x emissions are mostly due to the use phase of a catalytic converter.

Unlike the other key emissions, carbon dioxide is increased with the use of a catalytic converter. This result is expected. Referring back to Equation 1.2 on page 2, carbon dioxide is an output, along with carbon monoxide, from a typical engine. This is a key point because carbon dioxide is expected to be emitted by the engine alone, but the catalytic converter increases the carbon dioxide further because it is converting the carbon monoxide and hydrocarbons to carbon dioxide [2]. Carbon dioxide is by far the largest emission output to the environment compared to the three other emissions. While carbon dioxide is a gas monitored by the EPA voluntarily, it does not pose a direct short term threat to human health; however, carbon dioxide may pose a threat to long term human health. Totaling 35,940 kg per catalytic converter, the carbon dioxide emissions are 6,210 kg greater than those for a car without a catalytic converter. The use of gasoline is the primary supplier to this large emission total. As explained before, 8.92 kilograms of carbon dioxide are emitted due to one gallon of gasoline used. For a functional unit of 80,000 miles and a car with an average of 24 miles per gallon, this equates to a total of 3334 gallons of gasoline over the converter's lifetime. This yields an approximate total of 29,730 kg of carbon dioxide; this is the total CO_2 emission for the car without a catalytic converter. In addition to this amount, a total of 6183 kg of CO_2 are converted from CO. The extraction and processing of the catalytic converter create an additional 23.6 kg of carbon dioxide. Like the other key emissions, carbon dioxide emissions are the greatest during the use phase of the catalytic converter.

Carbon monoxide, hydrocarbons and nitrogen oxides emissions are all greatly lessened by the use of a catalytic converter. While this result is expected, the life cycle analysis provides evidence for this claim. Carbon dioxide emissions are increased because of a catalytic converter. This is also expected, but the life cycle analysis shows that most all of the emissions are due to the use of gasoline, not due to carbon monoxide and hydrocarbons converted or to the creation of the catalytic converter.

4.1.1 Sensitivity Analysis

Sensitivity analysis is used in this LCA to show whether or not an assumptions have a large effect on the outcome. The results of these five tests show that some assumptions have no effect, while some assumptions have small effects. Overall, this life cycle model is not very sensitive to the tested assumptions. This result is due to the fact that the life cycle is dominated by the use phase, and is therefore very sensitive to that.

Platinum and palladium are both used as an oxidation catalyst. Sometimes it is made with one or the other, and sometimes it is made with both. The driving force for the selection of the material used is the cost [40]. This sensitivity analysis compares the use of all platinum and all palladium to determine the environmental effects from manufacturing and processing the raw material. The results of the analysis show that there are no significant emission differences between the two tests. The changes in the emissions are so slight that the total emission is not even changed significantly. This is a good sign because the assumption of using all platinum does not have any impact on the life cycle. These results allow for platinum, palladium, to be interchanged without an influence on the emissions.

The second sensitivity analysis tests the assumption of alumina as the bulk of the washcoat. The results of this analysis indicate that this assumption does have a slight impact on the emission totals; hydrocarbon, nitrogen oxide and carbon monoxide emissions are not significantly affected by the changing of materials. Comparing all silica to half silica, half alumina, the carbon dioxide emissions are increased by 2.5 kg. The slight increases in emissions may be due to the fact that there are two extraction and manufacturing processes to account for; there may also be rounding errors within SimaPro causing the increases in emissions.

The cordierite processing energies were assumed to be the average processing energies of magnesia refractory brick. Sensitivity analysis is used to show whether or not taking 50% or 75% of the drying and firing processing energies will have an influence on the emissions produces. The results of this analysis show that there are slight decreases associated with halving these energies. There are also very slight decreases associated with taking 75% of the drying and firing energies. The results from this analysis indicates that since the use phase emissions are dominating the life cycle, only minor emission decreases are possible with changing the processing energies.

This life cycle assumed that microwave drying is used during the creation of the ceramic substrate. Sensitivity analysis is used to determine if using conventional drying will have an influence on the emissions produced. The results of this analysis show that there is a very small increase when using conventional drying instead of microwave drying. This result is expected because conventional drying is a longer process and requires more energy.

The last sensitivity analysis test is comparing the emissions produced from conventional firing to microwave firing. The assumption is that conventional firing methods are used. The results from this analysis show that there is a very small decrease in emissions between the two options. This is an expected result because microwave firing requires less energy.

4.2 Eco-indicator 99 (H)

Eco-indicator 99 (H) is a life cycle analysis tool used to show the damages caused to human health, ecosystem quality and resources. The damage comparisons can be seen in Figure 3.1. In this figure and the subsequent table, each damage category is compared side by side. Table 3.11 provides the actual damage in each category's unit. These numbers show that human health damage is decreased over 50%, and that ecosystem quality is decreased over 75% when a catalytic converter is used. The damage to resources is increased by 100% with a catalytic converter since the other model uses no resources. The decrease in human health damage directly correlates to less human lives lost and disabled. In the same manner, the decrease in ecosystem quality damage relates to less species lost, over an area, in a timespan. The increase in resource damage means that more energy will be required to acquire the resource in the future.

Tables 3.12, 3.13 and 3.14 provide the top three contributors to the human health damage, ecosystem quality damage and resource damage, respectively, for a car with a catalytic converter. For the human health damage category, the top three contributors are: emissions during use with the converter, platinum, and rhodium. The emissions during use with the converter are the majority, or 97.6%, of the human health damage. The platinum and rhodium have a combined 2.1% of the human health damage. The top three contributors to ecosystem quality are: emissions during use with the converter, platinum, and stainless steel. Like human health, emissions during use are 96.7% of the damage to ecosystem quality. The platinum and stainless steel have a combined ecosystem quality damage total of 2.4%. The top three contributors to resource damage are: stainless steel, platinum and rhodium. The stainless steel makes up 35.2% of the resources damage. The platinum has 24.5% of the resources damage, while the rhodium has 10.7% of the damage. These three materials make up 70.4% of the damages to resources. These results indicate that emissions during use are the dominant damage to human health and resources, while the damage to resources is spread out over various sources.

4.3 Cumulative Energy Demand

This single score analysis method is utilized to see exactly how much energy is being used to create a catalytic converter. The results show that about 260 MJ are used to create a single catalytic converter. The bulk of the energy, 229 MJ, comes from extraction and processing of the necessary materials. Almost 95% of this energy is due to stainless steel, platinum, rhodium, and corrugated board boxes. The stainless steel itself makes of 45.2% of the total material energy. While the loss of precious metals is important, the energy demand for the stainless steel resources is greater than the precious metals due to its larger mass. The other three materials make up 49.3% of the total material energy. Only 11.9% of the total energy is attributed to the processing of a catalytic converter.

Of the 260 MJ of total energy, 221 MJ is from a non-renewable, fossil energy source. Like the materials energy, the majority of the fossil energy is created from stainless steel, platinum, rhodium and corrugated board boxes. These four sources make up 82.7% of the total fossil energy. Overall, stainless steel, platinum and rhodium are the top three contributors to total energy usage. These three materials make up 76.3% of all energy used to produce a catalytic converter. It should be noted that the results are indicative of no recycling. The energies are assuming all virgin materials, but with recycling, these energies and the total energy could be reduced, as explained in section 2.5 Disposal. This is especially true since platinum and rhodium are large energy producers in the virgin state.

5.0 Conclusions

A life cycle analysis was used to determine the environmental impact of creating and using a catalytic converter in a car compared to not using a catalytic converter in a car. Two models were created in SimaPro so allow for a life cycle comparison of a car with and without a catalytic converter. These models were run and analyzed; they lead to the conclusion that a car with a catalytic converter impacts the environment less than a car without a catalytic converter in certain areas. The life cycle inventory showed that the carbon monoxide, hydrocarbon and nitrogen oxide emissions were decreased significantly in using a catalytic converter. Only carbon dioxide emissions were increased with the use of a catalytic converter, but this result was expected. The carbon dioxide emissions can be seen as an environmental issue because this pollutant is a greenhouse gas; it contributes to global warming potential, and has unknown long-term health effects. However, this result is an environmental benefit if considering that short term local atmospheric impacts, such as smog, are more important than long term global environmental impacts, such as global warming potential. Within the car with a catalytic converter, the emissions due to the use phase far exceeded the emissions due to the extraction and manufacturing phase. The life cycle analysis results showed that the damages to human health and ecosystem quality were significantly decreased with the use of the catalytic converter. Resource damage and energy required are two categories in which a car with a catalytic converter surpasses a car without a converter. Overall, this life cycle analysis concludes that a catalytic converter is a worthwhile environmental product for short term atmospheric benefits.

6.0 Future Work

Life cycle analysis has the potential to indicate whether or not a product is or is not environmentally friendly. This LCA showed that catalytic converters can be seen as a beneficial environmental product; however, future work can be done to improve this project. As a project continuation, this research suggests work in the following areas:

- Metal used for the substrate rather than cordierite ceramic.

While ceramic substrates have been more popular in the past, metal substrates are starting to emerge. An analysis could be done to compare metal versus ceramic as the material used for the substrate.

- Replace processing energies estimates.

The processing energies used in this analysis were compiled and estimated from various sources. This analysis could be greatly improved with actual energy usage data from the manufacturers.

- Processing of the metal catalyst.

The processing of the metal catalyst was left out of scope in this research. The addition of catalyst processing details would help to more fully encompass processing of the catalytic converter.

- Diesel or another form of fuel to power the vehicle.

It was assumed that the passenger car was fueled by gasoline in this research. Diesel catalytic converters are different from gasoline catalytic converters. Diesel converters also include a filter for particulate matter. An analysis could be done to show the similarities and differences between diesel and gasoline converters. Also, an analysis could include other forms of fueling such as biodiesel, electric and hybrid cars.

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Appendix A: Calculations

A.1 – Cordierite composition work:

The unbalanced equation of cordierite is:

$$Al_2(Si_2O_5)(OH)_4 + Mg_3(Si_2O_5)_2(OH)_2 + Al_2O_3 + Al(OH)_3 + SiO_2 \rightarrow \text{Cordierite} + \text{Water} \uparrow \quad (A.1)$$

where the inputs are: kaolin ($Al_2(Si_2O_5)(OH)_4$), talc ($Mg_3(Si_2O_5)_2(OH)_2$), alumina (Al_2O_3), aluminum hydroxide ($Al(OH)_3$), and silica (SiO_2). The weight percent of each input is known, from Table 2.2. For ease of calculation, it is assumed that there is a 100 gram sample. The results will be scaled up to correlate to the actual data. Table A.1 below gives the mass of each input compound for a 100 gram sample.

Table A.1: Masses of inputs for a 100 gram sample

Input Material	**Mass (gram)**
Kaolin	21.74
Talc	39.24
Alumina	11.23
Aluminum hydroxide	17.80
Silica	9.99
Total	100.0

These masses must be converted to moles. This is done by dividing the mass of the material by the molecular weight of the material. Table A.2 below determines the moles for each material.

Table A.2: Moles of material inputs for a 100 gram sample

Material	Mass (gram)		Molecular weight (g/mol)		Moles (mol)
Kaolin	21.74		258.157		0.084212
Talc	39.24		379.259		0.103465
Alumina	11.23	*divided by*	101.961	*equals*	0.11014
Aluminum hydroxide	17.80		78.003		0.228196
Silica	9.99		60.083		0.16627

These moles can then be used to determine the masses of each input element. To find these masses, the moles of the element (in the compound's formula) are multiplied by the moles of the compound material, which is then multiplied by the molecular weight of the element.

Table A.3: Masses of element inputs for a 100 gram sample

Material	Element	Moles of element (mol)	Moles of compound (mol)	Molecular weight of element (g/mol)	Mass of element (g)
Kaolin	Aluminum	2	0.084212	26.982	4.54
	Silicon	2	0.084212	28.085	4.73
	Oxygen	9	0.084212	15.999	12.13
	Hydrogen	4	0.084212	1.008	0.34
Talc	Magnesium	3	0.103465	24.305	7.54
	Silicon	4	0.103465	28.085	11.62
	Oxygen	12	0.103465	15.999	19.86
	Hydrogen	2	0.103465	1.008	0.21
Alumina	Aluminum	2	0.11014	26.982	5.94
	Oxygen	3	0.11014	15.999	5.29
Aluminum hydroxide	Aluminum	1	0.228196	26.982	6.16
	Oxygen	3	0.228196	15.999	10.95
	Hydrogen	3	0.228196	1.008	0.69
Silica	Silicon	1	0.16627	28.085	4.67
	Oxygen	2	0.16627	15.999	5.32

The totals for each element were found to be:

- Aluminum = 16.64 grams
- Silicon = 21.02 grams
- Magnesium = 7.54 grams
- Oxygen = 53.55 grams
- Hydrogen = 1.24 grams

These total input masses must be the same in the output. The masses are converted by taking the mass of the element, and dividing it by the molecular weight of the element. Table A.4 below gives the output moles of each element.

Table A.4: Moles of output elements for a 100 gram sample

Element	**Mass (gram)**		**Molecular weight (g/mol)**		**Moles (mol)**
Aluminum	16.64	*divided by*	26.982	*equals*	0.6169
Silicon	21.02		28.085		0.7486
Magnesium	7.54		24.305		0.3104
Oxygen	53.55		15.999		3.347
Hydrogen	1.24		1.008		1.228

The right side of equation A.1 can be broken down into output compounds. Equation A.2 provides this breakdown.

$$\text{Cordierite} + \text{Water} \longrightarrow Al_2O_3 + SiO_2 + MgO + H_2O \qquad \text{(A.2)}$$

The moles of each element, seen in Table A.4, can be used to determine the moles of each output compound. Referencing Equation A.2, there are two moles of aluminum in alumina; therefore, the moles of alumina are half of the moles of aluminum. This means that there are approximately 0.31 moles of alumina in a 100 gram sample. In the same manner, there is one mole of silicon in silica; therefore, the moles of silica are equal to the moles of silicon. This means that there is 0.75 moles of silica in a 100 gram sample. There is one mole of magnesium in magnesia, so there are equal moles of magnesia and magnesium. From this, it is known that there is 0.31 moles of magnesia in a 100 gram sample. Finally, there are two moles of hydrogen in water. The moles of water are half of the moles of hydrogen; this is 0.61 moles of water in a 100 gram sample. All of these numbers can be checked by verifying the moles of the oxygen. Equation A.3 below shows this verification. The result of Equation A.3 matches the oxygen mole value found in Table A.4 above

$$(\text{mol } Al_2O_3 \times \text{mol O}) + (\text{mol } SiO_2 \times \text{mol O}) + (\text{mol MgO} \times \text{mol O}) + (\text{mol } H_2O \times \text{mol O})$$

$$(0.31 \times 3) + (0.75 \times 2) + (0.31 \times 1) + (0.61 \times 1) = 3.35 \tag{A.3}$$

Equation A.2 can now be modified to include the balanced mole count. This can be seen in Equation A.4 below.

$$\text{Cordierite} + \text{Water} \longrightarrow 0.31\ Al_2O_3 + 0.75\ SiO_2 + 0.31\ MgO + 0.61\ H_2O \tag{A.4}$$

This equation can be modified by dividing all coefficients 0.31 to give the following equation:

$$\text{Cordierite} + \text{Water} \longrightarrow Al_2O_3 + 2.5\ SiO_2 + MgO + 2.03\ H_2O \tag{A.5}$$

This equation can again be modified by multiplying all coefficients 2 to give the following equation:

$$\text{Cordierite} + \text{Water} \longrightarrow 2\ Al_2O_3 + 5\ SiO_2 + 2\ MgO + 4.07\ H_2O \tag{A.6}$$

Equation A.6 shows that the composition found in Tables 2.2 and A.1 provides the expected cordierite composition, seen in section 1.1.3, of two parts alumina, two parts magnesia and five parts silica.

The moles calculated from the data in Table A.4 can be used to determine the masses of each output compound. This is done in Table A.5 below.

Table A.5: Masses of output compounds for a 100 gram sample

Material	**Moles (mol)**		**Molecular weight (g/mol)**		**Mass (gram)**
Alumina	0.31	*multiplied by*	101.961	*equals*	31.6
Silica	0.75		40.304		12.5
Magnesia	0.31		60.083		45.0
Water	0.61		18.015		10.9

From this table, it is determined that of the initial 100 gram sample, cordierite is 89.1 grams, and water is 10.9 grams.

This data must be scaled up to be used with the experimental data in this analysis. The output cordierite was measured to be 832.3 grams. This number and Table A.5 can be used to determine the output water. Equation A.7 below determines the total output mass, where 'x' is the total output mass.

$$832.3 \text{ grams of cordierite} + 10.9\% (x) = x \qquad (A.7)$$

Solving for 'x', the total output mass is found to be 935.169 grams. From this, the amount of output water is determined in Equation A.8 below. The percent of water is multiplied by the total output mass.

$$10.9\% (935.169 \text{ grams}) = 102.768 \text{ grams} \qquad (A.8)$$

The remaining output compounds are scaled up to the experimental data by dividing the mass of each compound by the total cordierite mass for the 100 gram sample. This number is then multiplied by the total cordierite mass for the experimental data. Table A.6 below gives the conversion for the 100 gram sample to the experimental data.

Table A.6: Masses of output compounds for experimental data

Material	**Percent contribution**	**Experimental Cordierite mass (grams)**	**Experimental mass of output compound (grams)**
Alumina	$\left(\frac{31.6}{89.1}\right) = 0.36 \times 100\% = 35.5\%$	832.2	295.431
Silica	$\left(\frac{45.0}{89.1}\right) = 0.50\ \times 100\% = 50.5\%$	832.2	420.261
Magnesia	$\left(\frac{12.5}{89.1}\right) = 0.14 \times 100\% = 14\%$	832.2	116.508

These masses can be converted back to moles to determine the moles of the inputs. Table A.7 below determines the moles of output compounds for the experimental data.

Table A.7: Moles of output compounds for experimental data

Material	**Mass (gram)**		**Molecular weight (g/mol)**		**Moles (mol)**
Alumina	295.431		101.961		2.9
Silica	420.261	*divided by*	60.083	*equals*	6.9
Magnesia	116.508		40.304		2.9
Water	102.768		18.015		5.7

The output moles for the experimental data are about 9.35 times greater than the output moles for the 100 gram sample. This factor can be applied to the input moles for the 100 gram sample to determine the input moles for the experimental data. Equation A.9 below gives the balanced equation for the 100 gram sample.

$$0.08\ Al_2(Si_2O_5)(OH)_4 + 0.10\ Mg_3(Si_2O_5)_2(OH)_2 + 0.11\ Al_2O_3 + 0.23\ Al(OH)_3 + 0.17\ SiO_2 \rightarrow 0.31\ Al_2O_3 + 0.75\ SiO_2 + 0.31\ MgO + 0.61\ H_2O \quad \text{(A.9)}$$

This equation can be scaled up for the experimental data by the multiplying the mole of each compound by the factor determined above, 9.35. This can be seen in equation A.10 below.

$$0.75\ Al_2(Si_2O_5)(OH)_4 + 0.94\ Mg_3(Si_2O_5)_2(OH)_2 + 1.0\ Al_2O_3 + 2.2\ Al(OH)_3 + 1.6\ SiO_2 \rightarrow 2.9\ Al_2O_3 + 7.0\ SiO_2 + 2.9\ MgO + 5.7\ H_2O \quad \text{(A.10)}$$

The moles of the input compounds can be converted into masses by multiplying the moles by the molecular weight of the input compounds. This conversion can be seen in Table A.8 below. These masses will be input into SimaPro for the car with a catalytic converter model.

Table A.8: Masses of input compounds for experimental data

Material	**Moles (mol)**		**Molecular weight (g/mol)**		**Mass (gram)**
Kaolin	0.75		258.157		193.62
Talc	0.94	*multiplied by*	379.259		356.50
Alumina	1.0		101.961	*equals*	101.96
Aluminum hydroxide	2.2		78.003		171.61
Silica	1.6		60.083		96.13

A.2 – Washcoat mass calculation

The washcoat is 100 parts by weight alumina and 4 parts by weight rare earth element oxide are suspended in 250 parts by weight of water. The washcoat is 25 weight percent of the cordierite substrate. The sample substrate was weighed at 1114.04 grams; therefore, the washcoat is 278.51 or 25 weight percent of the substrate.

A.3 – Vehicle emission calculations

Table A.9 below gives the vehicle emissions in grams per mile. The emissions converted are also included. As stated in the assumptions, the nitrogen oxides converted are negligible in this study.

Table A.9: Vehicle emissions

	Carbon monoxide (g/mi)	Hydrocarbons (g/mi)	Nitrogen oxides (g/mi)
Car without a catalytic converter	43.5	4.5	2.74
Car with a catalytic converter	3.22	0.3	0.644
Emissions converted	40.2	4.2	2.09

Table A.10 below determines the carbon dioxide emissions due to gasoline. This emission amount is the total carbon dioxide emissions in the car without a catalytic converter. The car with a catalytic converter will add this emission amount, plus the converted amounts from Table A.9, plus any carbon dioxide emissions from extraction and processing.

Table A.10: Carbon dioxide emissions due to gasoline

Carbon dioxide emissions	
8.92	kilograms CO2 per gallon of gasoline
divided by	
24	miles per gallon
Equals	
0.371667	kilograms CO2 per mile
Times	
80000	miles (functional unit)
Equals	
29733.33	kilograms of CO2

Table A.11 below provides the vehicle emissions in grams per mile for carbon dioxide. This table has the converted hydrocarbon and carbon monoxide emissions as well as the emissions due to gasoline.

Table A.11: Carbon dioxide emissions

	Carbon dioxide (g/mi)
CO emissions converted	63.162
HC emissions converted	14.130
Gasoline	371.667
Total	448.958

Table A.12 below calculates the emissions for the pollutants for a car with and without a catalytic converter. The emission in grams per mile is multiplied by the functional unit, giving a total in grams. The grams are then converted to kilograms.

Table A.12: Pollutant emission calculations

Pollutant	**Emission**	**Unit**	**Functional Unit**	**Pollutant**	**Emission**	**Unit**
CO	43.5	g/mi		CO	3480	kg
HC	4.5	g/mi		HC	360.8	kg
NOx	2.74	g/mi		NOx	219.2	kg
CO	3.22	g/mi	* 80000 miles =	CO	257.6	kg
HC	0.3	g/mi		HC	25.76	kg
NOx	0.644	g/mi		NOx	51.52	kg
CO converted to CO2	63.162	g/mi		CO converted to CO2	5052.943	kg
HC converted to CO2	14.130	g/mi		CO converted to CO2	1130.395	kg

A.4 – Microwave firing calculations:

The range given for conventional drying and firing is 3.0 – 6.3 MJ/kg. Using the energies for conventional drying and firing of refractories, a total energy can be found. Equation A.11 provides the total energy for these processes. Equation A.12 gives the conventional drying as a percentage of the total energy.

Total conventional energy for a refractory = Refractory conventional drying energy + Refractory conventional firing energy

$$Total\ conventional\ energy\ for\ a\ refractory = 10.87 \text{ x } 10^6 \text{ kW} \cdot \text{h/yr} + 38.53 \text{ x } 10^6 \text{ kW} \cdot \text{h/y} = 49\text{x } 10^6 \text{ kW} \cdot \text{h/yr} \quad \text{(A.11)}$$

$$Conventional\ Drying\ Percentage = \frac{10.87\text{x } 10^6 \text{ kW·h/yr}}{49.4\text{x } 10^6 \text{ kW·h/yr}} \times 100\% = 22.00\% \quad \text{(A.12)}$$

This percentage can be applied to the given range for drying and firing to show how much is the drying itself. Applying 22% to the drying, firing range of 3.0 – 6.3 MJ/kg yields a drying range of 0.66 – 1.386 MJ/kg. The remaining 2.34 – 4.914 MJ/kg is the range for conventional firing of a refractory.

Referencing Table 2.7 on page 30, the conventional firing and microwave firing can be compared. Equation A.13 gives the microwave firing energy as a percentage of conventional firing energy.

$$Microwave\ Firing\ Percentage = \frac{3.85\text{x } 10^6 \text{ kW·h/yr}}{38.53\text{x } 10^6 \text{ kW·h/yr}} \times 100\% = 9.992\% \quad \text{(A.13)}$$

This percentage can be applied to the conventional firing range, 2.34 – 4.914 MJ/kg, to find the microwave firing range. This range is found to be 0.2338 – 0.4910 MJ/kg. Since this range is characteristic of refractories, and not specifically cordierite, the average value, 0.7248 MJ/kg, is used in the analysis.

Appendix B

Table B.1: Emission Totals

Carbon dioxide (kg)		
Use		35920
Manufacturing	CO2 biogenic	0.546
	CO2 fossil	7.63
	CO2 in air	1.49
	CO2 land transformation	14
	Total	23.666

Carbon monoxide (kg)		
Use		258
Manufacturing	CO2 biogenic	0.147
	CO2 fossil	0.0447
	Total	0.1917

Hydrocarbons (kg)		
Use		25.8
Manufacturing	Hydrocarbons, aliphatic, alkanes, cyclic	0.000000133
	Hydrocarbons, aliphatic, alkanes, unspecified, air	0.0000275
	Hydrocarbons, aliphatic, alkanes, unspecified, water	0.00000281
	Hydrocarbons, aliphatic, unsaturated, air	0.0000069
	Hydrocarbons, aliphatic, unsaturated, water	0.000000259
	Hydrocarbons, aromatic, air	0.0000531
	Hydrocarbons, aromatic, water	0.0000121
	Hydrocarbons, chlorinated	0.000000412
	Hydrocarbons, unspecified, water	0.0000924
	Total	0.000158012

Nitrogen Oxides (kg)	
Use	51.5
Manufacturing	0.1