CATALYTIC CONVERTER THERMAL MODEL FOR HYBRID ELECTRIC VEHICLE ENGINE ON/OFF CONTROL STRATEGY DEVELOPMENT

by

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ABSTRACT

A 3-dimensional (3-D), thermochemical catalytic converter model was developed to investigate the effects of engine-off periods typical in hybrid electric vehicle (HEV) operation on overall emissions conversion effectiveness. The model includes a 3-reaction mechanism to account for the majority of heat generation due to exhaust species chemical conversion during engine operation. The modeled cross-sectional area of the catalytic converter was decreased to reduce computational complexity. This simplification resulted in an over prediction of shell heat loss to the surroundings due to the incorrect shell surface area to volume ratio. Therefore, an adiabatic assumption was used to analyze the substrate’s thermal behavior without the influence of external heat transfer. The analytical model was experimentally validated with an engine that provided feedgas to a catalytic converter. The catalytic converter was instrumented with thermocouples for internal and surface temperature measurement. The reduced-size, catalytic converter model with the adiabatic assumption produced mid-catalytic converter temperature predictions within 3%. However, thermal behavior during engine-off period could not be predicted since radial heat transfer was eliminated with the adiabatic assumption but is the dominating effect in real cool-down. Accurate temperature predictions during cool-down requires modeling a realistic surface area to volume ratio which is outside of the computational limitations of the modeling platform used in this work.
# LIST OF ABBREVIATIONS AND SYMBOLS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-D</td>
<td>0-dimensional</td>
</tr>
<tr>
<td>1-D</td>
<td>1-dimensional</td>
</tr>
<tr>
<td>3-D</td>
<td>3-dimensional</td>
</tr>
<tr>
<td>APP</td>
<td>Accelerator pedal position</td>
</tr>
<tr>
<td>CAA</td>
<td>Clean Air Act</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational fluid dynamics</td>
</tr>
<tr>
<td>C₃H₆</td>
<td>Propene</td>
</tr>
<tr>
<td>C₃H₈</td>
<td>Propane</td>
</tr>
<tr>
<td>CO</td>
<td>Carbon monoxide</td>
</tr>
<tr>
<td>CO₂</td>
<td>Carbon dioxide</td>
</tr>
<tr>
<td>CO₂-e</td>
<td>Carbon dioxide equivalent</td>
</tr>
<tr>
<td>DAQ</td>
<td>Data acquisition</td>
</tr>
<tr>
<td>DC</td>
<td>Direct-current</td>
</tr>
<tr>
<td>ECL</td>
<td>Engines and Combustion Laboratory</td>
</tr>
<tr>
<td>ECM</td>
<td>Engine control module</td>
</tr>
<tr>
<td>EPA</td>
<td>Environmental Protection Agency</td>
</tr>
<tr>
<td>EV</td>
<td>Electric vehicle</td>
</tr>
<tr>
<td>GHG</td>
<td>Greenhouse gas</td>
</tr>
<tr>
<td>GM</td>
<td>General Motors</td>
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</table>
HC  Hydrocarbon
HEV  Hybrid electric vehicle
HIL  Hardware-in-the-loop
MY   Model year
NI   National Instruments
NOx  Oxides of nitrogen
Pd   Palladium
Pt   Platinum
Rh   Rhodium
UA   The University of Alabama
UHC  Unburned hydrocarbon
A    Pre-exponential factor
$A$  Cross-sectional area of the gas element
$a_j$ Catalyst surface area per unit volume of substrate
$c_1$ Integration constant
$c_2$ Integration constant
$c_g$ Total gas concentration
$C_i$ Concentration of species, $i$
$c_{p,gas}$ Specific heat of gas in element, $i,j,k$
$c_{p,sub}$ Specific heat of substrate element, $i,j,k$
$D_h$ Hydraulic diameter
$D_i$ Diffusion mass transfer coefficient of species, $i$ (for general equation)
\( D_{i,m} \) Mass diffusivity

\( E_a \) Activation energy

\( \Delta H \) Enthalpy of reaction

\( h_{\text{ext}} \) External convection coefficient

\( h_{\text{ext,free}} \) External natural convection coefficient

\( h_{\text{int}} \) Internal convection coefficient

\( h_{\text{int,free}} \) Internal natural convection coefficient

\( k_{\text{gas}} \) Thermal conductivity of gas in element, i,j,k

\( k_{\text{mi}} \) Diffusion mass transfer coefficient of a species from the gas element to the substrate element

\( k_{\text{wall}} \) Thermal conductivity of substrate wall in element i,j,k

\( l \) Cross-sectional length of the gas element

\( m_{\text{gas}} \) Mass of the gas in element i,j,k

\( m_{\text{sub}} \) Mass of substrate element, i,j,k

\( \dot{m}_{\text{air}} \) Mass flow rate of engine intake air

\( \dot{m}_{\text{exhaust}} \) Mass flow rate of engine-out exhaust gas

\( \dot{m}_{\text{fuel}} \) Mass flow rate of fuel

\( \dot{m}_{\text{gas}} \) Mass flow rate of gas in element, i,j,k

\( M \) Matrix of temperature coefficients

\( M_i \) Molecular weight of species, i

\( M_{\text{N2}} \) Molecular weight of N\(_2\)

\( N \) Number of channels in the real catalytic converter

\( Nu \) Nusselt number

\( P \) Absolute pressure
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>$\tilde{q}$</td>
<td>Heat flux</td>
</tr>
<tr>
<td>$\dot{Q}_{\text{gen}}$</td>
<td>Rate of heat generation</td>
</tr>
<tr>
<td>$R_{\text{eq, gas}}$</td>
<td>Thermal equivalent resistance for gas to substrate elements</td>
</tr>
<tr>
<td>$R_{\text{eq, sub}}$</td>
<td>Thermal equivalent resistance for substrate to substrate elements</td>
</tr>
<tr>
<td>$R_{\text{eq, sub-steel}}$</td>
<td>Thermal equivalent resistance for substrate to steel elements</td>
</tr>
<tr>
<td>$R_{\text{eq, sub-steel}}$</td>
<td>Thermal equivalent resistance for steel elements to air</td>
</tr>
<tr>
<td>$R_i$</td>
<td>Generation of species, i, from chemical reactions</td>
</tr>
<tr>
<td>$r_j$</td>
<td>Reaction rate of reaction, j</td>
</tr>
<tr>
<td>$R_{\text{major}}$</td>
<td>Catalytic converter major axis radius</td>
</tr>
<tr>
<td>$R_{\text{minor}}$</td>
<td>Catalytic converter minor axis radius</td>
</tr>
<tr>
<td>$R_u$</td>
<td>Universal gas constant</td>
</tr>
<tr>
<td>$S$</td>
<td>Ratio of the void cross-sectional area per unit volume substrate</td>
</tr>
<tr>
<td>$S_h$</td>
<td>Sherwood number</td>
</tr>
<tr>
<td>$s_{i,j}$</td>
<td>Stoichiometric coefficient for species, i, of reaction, j</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>Time step</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$[T]$</td>
<td>Temperature array</td>
</tr>
<tr>
<td>$T$</td>
<td>Absolute Temperature</td>
</tr>
<tr>
<td>$T_{i,j,k}$</td>
<td>Absolute temperature at element location, i,j,k</td>
</tr>
<tr>
<td>$t_{\text{wall}}$</td>
<td>Substrate element wall thickness</td>
</tr>
<tr>
<td>$\hat{v}$</td>
<td>Velocity field</td>
</tr>
<tr>
<td>$w$</td>
<td>Total molar flow rate</td>
</tr>
<tr>
<td>$X$</td>
<td>Arbitrary species concentration</td>
</tr>
</tbody>
</table>
\( x_s \)  
Mole fraction of species in the substrate element

\( x_g \)  
Mole fraction of species in the gas element

\( Y \)  
Arbitrary species concentration

\( \Delta z \)  
Length step size in axial direction

\( z \)  
Axial length of catalytic converter

\( \bar{z} \)  
Axial length of one element

\( \sum_i \)  
Diffusivity volume of species, \( i \)

\( \rho_{gas} \)  
Density of gas in element

\( \rho_{sub} \)  
Density of substrate element

\( \Phi \)  
Equivalence ratio
ACKNOWLEDGEMENTS

It is my sincere hope that these acknowledgements are not overlooked because the contents of this thesis would be painfully bare if not for the support of several faculty members in the College of Engineering at The University of Alabama.

I especially want to thank my advisor, committee chair, and most importantly teacher, Dr. Paul Puzinauskas, for his relentless belief in me and the work that I do. I am forever indebted to his expertise in the thermal sciences and his undying effort to pass the knowledge to me. I also want to thank Dr. Bittle immensely for the support he provided me as a member of this thesis committee and beyond. Dr. Bittle’s perspectives and questioning greatly benefited the final outcome of this thesis. And of course, I must thank Dr. Lane, who I did not have the pleasure of knowing sooner, but provided invaluable insight into the chemical phenomena related to this thesis. Finally, thank you to all of the people that helped behind the scenes, especially Dr. Ashford and Allen Loper. All of you have unsurpassably served as confidants who taught me indispensable lessons that I will continue to use throughout my career and life.
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CHAPTER 1
INTRODUCTION

1.1. Catalytic Converter Conception to Widespread Adoption

French mechanical engineer, Eugene Houdry, patented the catalytic converter in 1950 for on-board reduction of pollutants from gasoline engines (Scoltock, 2013). The invention was before its time in the sense that there would not be legislation to regulate tailpipe pollutants for another 20 years. Houdry’s patent reads “This invention relates to internal combustion engines and more particularly to methods and means for treating the exhaust products of the same, specifically for effecting oxidation of burnable components and for rendering harmless and non-offensive toxic as well as malodorous materials and compounds in the exhaust gases of such engines” (Scoltock, 2013). The adoption of the catalytic converter for mainstream use was spurred by the U.S. legislation that followed the Clean Air Act (CAA) of 1970. The CAA gave federal-level authority to regulate air pollutants from mobile and stationary emissions’ sources, and required a 90% reduction in tailpipe emissions from automobiles by 1975 (EPA, 2017). The U.S. Environmental Protection Agency (EPA) was established virtually concurrently to the CAA and set the first National Air Quality Standards in 1971 (EPA, 2017). In response to the EPA’s newly formulated emissions’ standards, General Motors (GM) announced in a 1974 news article that all vehicles in the 1975 fleet would come equipped with a catalytic converter (“General Motors Believes…”, 1974). Other automotive manufacturers soon followed, and the catalytic converter became widespread.
1.2. How a Catalytic Converter Works

The first catalytic converters were referred to as two-way catalytic converters and worked to decrease carbon monoxide (CO) and hydrocarbon (HC) pollutants from engine-out exhaust gas. The three-way catalytic converter was later developed to also reduce oxides of nitrogen (NOx).

Figure 1.1. Catalytic Converter Depiction

Figure 1.1 illustrates general catalytic converter operation. Engine-out exhaust gas flows into the catalytic converter which houses an underlying, typically ceramic, structure called the substrate. The densely packed substrate channels are covered in a washcoat that maximizes surface area and houses the precious metal particles. A single channel consisting of the substrate that effectively creates the channel, the washcoat, and the precious metal catalysts is portrayed in Figure 1.2.
The global conversion of the engine-out emissions to tailpipe emissions is governed by complex chemical kinetics that includes multiple elementary reactions. A subset of those reactions is shown in Table 1.1. The precious metals (typically Platinum, Palladium, & Rhodium) are the catalysts for the oxidation and reduction reactions. Freyschlag et al. describe a catalyst as “… a substance that facilitates a chemical transformation without itself being consumed in the process; this power has a mysterious, almost magic-wand character.”
Table 1.1.


<table>
<thead>
<tr>
<th></th>
<th>Reaction</th>
<th>Reaction Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CO + 0.5O₂ → CO₂</td>
<td>Oxidation</td>
</tr>
<tr>
<td>2</td>
<td>C₃H₆ + 4.5O₂ → 3CO₂ + 3H₂O</td>
<td>Oxidation</td>
</tr>
<tr>
<td>3</td>
<td>C₃H₈ + 5O₂ → 3CO₂ + 4H₂O</td>
<td>Oxidation</td>
</tr>
<tr>
<td>4</td>
<td>H₂ + O₂ → H₂O</td>
<td>Oxidation</td>
</tr>
<tr>
<td>5</td>
<td>CO + NO → CO₂ + 0.5N₂</td>
<td>NO Reduction</td>
</tr>
<tr>
<td>6</td>
<td>C₃H₆ + 9NO → 3CO₂ + 3H₂O + 4.5N₂</td>
<td>NO Reduction</td>
</tr>
<tr>
<td>7</td>
<td>H₂ + NO → H₂O + 0.5N₂</td>
<td>NO Reduction</td>
</tr>
<tr>
<td>8</td>
<td>CO + H₂O ↔ CO₂ + H₂</td>
<td>Water-Gas and Steam Reforming</td>
</tr>
<tr>
<td>9</td>
<td>C₃H₆ + 3H₂O → 3CO + 6H₂</td>
<td>Water-Gas and Steam Reforming</td>
</tr>
<tr>
<td>10</td>
<td>2Ce₂O₃ + O₂ → 4CeO₂</td>
<td>Ceria (Oxygen Storage)</td>
</tr>
<tr>
<td>11</td>
<td>Ce₂O₃ + NO → 2CeO₂ + 0.5N₂</td>
<td>Ceria (Oxygen Storage)</td>
</tr>
<tr>
<td>12</td>
<td>CO + 2CeO₂ → Ce₂O₃ + CO₂</td>
<td>Ceria (Oxygen Storage)</td>
</tr>
<tr>
<td>13</td>
<td>C₃H₆ + 12CeO₂ → 6Ce₂O₃ + 3CO + 3H₂O</td>
<td>Ceria (Oxygen Storage)</td>
</tr>
<tr>
<td>14</td>
<td>C₃H₈ + 14CeO₂ → 7CeO₂ + 3CO + 4H₂O</td>
<td>Ceria (Oxygen Storage)</td>
</tr>
<tr>
<td>15</td>
<td>H₂ + 2CeO₂ → Ce₂O₃ + H₂O</td>
<td>Ceria (Oxygen Storage)</td>
</tr>
</tbody>
</table>

Of the several elementary reactions occurring for a given species, the reaction with the lowest activation energy proceeds first. The catalyst works to lower the activation energy even further. The activation energy appears in the Arrhenius equation which determines the rate constant, \( k \), for a certain reaction:

\[
k = A e^{-\frac{E_a}{RT}} \tag{1.1}
\]

where

A is the pre-exponential factor

\( E_a \) is the activation energy
R is the gas constant

T is the absolute temperature

The reaction rate is then calculated as a function of the rate constant and species concentration.

The reaction rate of a first-order reaction is:

\[ r = k[X][Y] \]

where

X and Y are species concentrations

Light-off is a global phenomenon and refers to the temperature at which 50% of engine-out pollutant species are converted (Ashford, 2006). The reaction rate(s) that occurs first therefore determine(s) light-off. Since modern catalytic converters are typically 98-99% effective at reducing pollutants after light-off, the majority of emissions in a drive cycle occur in the first 60-90 seconds after a cold start. In fact, 60-95% of total hydrocarbons are emitted in that time period (Ashford, 2006). As a result of many years of research, modern catalytic converters achieve light-offs typically under 15 seconds.

These advances in catalytic converter performance coupled with improvements in engine-out emissions have nearly eliminated concerns regarding light-duty passenger vehicles’ contribution to criteria emissions. However, recently growing climate change concerns have refocused engine development efforts on reduction of greenhouse gas (GHG) emissions. Improvements in gasoline engine efficiency result in proportional reductions in CO₂ emissions which constitute a significant portion of anthropogenic GHG emissions. The EPA has set model year (MY) 2025 CO₂ emissions standards to 173 grams per mile or 51.4 MPG-e for light-duty passenger vehicles. This standard is estimated to result in a total reduction of 540 million metric
tons (CO\textsubscript{2}-e) of GHG and 1.2 billion barrels of oil over the lifetime of MY 2022-2025 vehicles as shown in Figure 1.3 (EPA, 2017).

![Figure 1.3. Trends in Reduction in CO2 Emissions 2012-2025 (expected) (EPA, 2017)](image)

The EPA projects these targets will be met primarily through advanced gasoline vehicle technologies. However, they estimate 25% of an automaker’s fleets will require some level of vehicle electrification (EPA, 2017). Automotive manufacturers have already responded by introducing hybrid electric vehicles (HEVs) and purely electric vehicles (EVs) into their fleets. On January 3, 2017, Ford Motor Company confirmed seven electrified vehicles to hit the market by MY 2020 including the top-selling F-150 and Mustang (“Ford Adding Electrified…”, 2017).

HEV operation typically has battery charge depleting (i.e. engine-off) periods when the vehicle is relying solely on the on-board electric motors for propulsion. Moreover, many HEVs and modern conventional vehicles employ ultra-efficient and/or lean combustion strategies
which characteristically feature lower exhaust temperatures. Because operation above light off
temperature is essential for optimal performance of a catalytic converter, engine-off periods and
relatively low temperature exhaust pose significant threats to its overall effectiveness over the
course of a drive cycle. The objective of this thesis is to develop and validate a catalytic
converter model for future investigation of the effects of past and present engine operation to
determine how a given hybrid control strategy will affect total criteria tailpipe emissions.
The goal of catalytic converter design is to achieve quick light-offs and heat retention without over-heating to meet regulated criteria tailpipe emissions for the warranted lifetime of the catalytic converter (typically 150,000 miles). Catalytic converter operation is contingent on its design, proximity to the engine, and the feedgas temperature and composition determined by engine operating conditions. The operationally influential parameters specific to catalytic converter design include overall geometry, channel density, substrate wall thickness, insulation thickness, and catalyst loading. Numerous models have been created to help elucidate the underlying physics and influential parameters that govern catalytic converter operation. The analytical model developed in this thesis instead focuses on the thermochemical behavior of catalytic converter itself with respect to dynamic boundary conditions determined by engine operation. The goal of this work is to model an existing catalytic converter to understand the influence of vehicle-level control strategies on the catalytic converter effectiveness during drive cycles. The purpose of this literature review is to determine the applicability of existing models to the objectives of this thesis.

The multitude of gas flow channels within a catalytic converter substrate present challenging tradeoffs between model complexity and accuracy in results. Most existing models make geometrical simplifications to predict trends without modeling the entirety of the channels; often, only a single channel is modeled.
Michel et al. developed a 0-D model that used detailed, catalytic converter specific maps of emissions’ conversion efficiencies. The conversion efficiencies are obtained from experimental data and are represented as a function of exhaust gas flow rate and mid-catalytic converter temperature. A map of CO conversion efficiency used by Michel et al. for this model is displayed in Figure 2.1.

![Figure 2.1. CO Conversion Efficiency Map (Michel, 2015)](image)

This approach significantly reduces computational complexity as only a single temperature prediction within the catalytic converter is required. Moreover, the complex chemical kinetics need not be modeled with this approach. Reducing computational complexity was especially important because the emissions predictions were used in a supervisory controller to optimize fuel consumption and tailpipe emissions in a gasoline-HEV. This application is nearly identical to the proposed application of the model presented in this thesis; however, the authors did not note if the model accurately predicted temperature during engine-off conditions.
The model was only validated while the engine was operating and motoring. Moreover, the 0-D type model required catalytic converter-specific, time-intensive experimental tests to obtain the necessary maps of emissions’ conversion efficiencies.

Single-channel (1-D) models are commonly used in literature to reduce computational complexity. A single-channel model was used by Ramanathan et al. to estimate kinetic parameters specific to 3-way catalytic converters. The authors noted the model was limited to predicting light-off. Furthermore, Aslanjan et al. showed multi-channel models to be more accurate than single-channel models because the radial temperature distribution can be accounted for in multi-channel models. The radial temperature distribution is important for accurate emissions predictions during warm-up (engine-on) since the catalytic reactions are especially sensitive to temperature. Still, for warm-up, the added complexity comes with little added benefit in accuracy. The authors did not consider comparison in accuracy for single and multi-channel models during cool-down (engine-off). The thermal behavior of the catalytic converter during cool-down is sparsely studied in literature. It is anticipated, however, that a multi-channel model is necessary to predict cool-down trends since heat transfer is predominantly via radial conduction. In fact, Hosoi et al. showed axial heat transfer to be nearly negligible during cool-down as illustrated by Figure 2.2. Inversely, axial heat transfer during warm-up is the dominant effect as shown in Figure 2.3. Since the thermal behavior of the catalytic converter during cool-down is critical for the intended HEV control strategy application, the single-channel approach is not appropriate.
The aforementioned Hosoi et al. model was a 3-D approach that accurately predicted both axial and radial temperature distributions during warm-up and cool-down simulations. Their model differentiated between substrate and gas channel thermal behavior by modeling separate control volumes with the respective energy equations as shown in Figure 2.4.
The model was used to improve fuel consumption during engine restart after a short parking period. The behavior of the catalytic converter during parked conditions will be similar to its behavior during the engine-off periods in HEVs when the vehicle is propelled solely by electric motors. The difference, of course, is the cooling effect on the shell due to forced convection versus natural convection. The Hosoi et al. model could be used to meet the desired goals of this thesis, but was developed by Toyota Motor Corporation and therefore not accessible in the public domain.

Other 3-D catalytic converter models exist in literature, but are mostly developed in commercial computational fluid dynamics (CFD) software to analyze the complex fluid behavior. Though the fluid behavior does indeed affect thermal behavior, the predominant flow effect is due to the gas’s velocity distribution at the front face of the catalytic converter. The
effect of the cross-sectional area ratio (inlet area to substrate area) on velocity distribution was studied by Jeong et al. and is illustrated in Figure 2.5.

![Figure 2.5](image)

**Figure 2.5. Effect of Cross-sectional Inlet to Brick Area Ratio on Inlet Velocity Distribution**

This behavior can only be predicted by modeling the full exhaust line from the engine manifold to the catalytic converter. Jeong et al. split their computational model into separate groups: a group for the flow region pre-catalytic converter and a group for the flow region within
the substrate. The authors assumed fully developed laminar flow within the substrate, whereas the flow domain outside the substrate was assumed unsteady, compressible, axisymmetric three-dimensional turbulent flow. Modeling the flow domain outside the substrate required solving the Navier Stokes equations. Finally, to investigate the effects of the velocity distribution entering the substrate on the substrate’s thermal behavior, three-dimensional turbulent flow and heat and mass transfer equations with chemical reactions had to be solved simultaneously. While this approach is comprehensive, the complexity associated with a full CFD solution with a reacting flow makes it impractical for the intended application to integrate the model into a dynamic vehicle controls system.

As noted by Hosoi et al., the thermal behavior of the catalytic converter during cool-down is only is sparsely studied, and therefore models suitable to predict those trends are limited. The models that would be suitable are either too computationally expensive for the application or not available to the public. As such, a 3-D model was developed to predict both warm-up and cool-down trends for intended use in a HEV supervisory controller. The analytical model developed in this thesis exists as a source code rather than commercial CFD software for ease of integration into a pre-existing HEV supervisory controller in Simulink.
CHAPTER 3
METHODOLOGY

This chapter is comprised of two subsections which respectively detail the analytical modeling and experimental methods used to meet the aforementioned thesis objectives. The thermo-chemical catalytic converter model was developed to predict the thermal state of the catalytic converter substrate during dynamic vehicle simulations used to optimize HEV control strategies. A major challenge in these operational strategies is to maintain conversion effectiveness during periods when the engine is off or running under conditions of ultra-low exhaust temperatures. The experimental effort was conducted to verify the relationship between the substrate’s thermal state and its performance and to acquire data for model validation.

3.1. Mathematical Model

The primary goal of the mathematical model was to predict radial and axial temperature distribution (and therefore conversion effectiveness) in a catalytic converter with respect to time and boundary conditions. The initial and boundary conditions were determined from engine operation history and ambient conditions. The approach included discretizing the energy equation and accounting for heat generation due to engine-out exhaust species conversion.

Two distinct control volumes were considered for mathematical modeling: a substrate element and a gas channel element. A discretized solution to the unsteady three-dimensional energy equation was developed for both types of control volumes. This approach allows
distinction between the thermal behavior of the gas and the substrate elements while accounting for thermal interactions and mass transfer between the two.

The following topics will be covered in the remainder of this section: Assumptions Overview, Development of Energy Equation for a Gas Element, Development of Energy Equation for Substrate Element, Solution Process Overview, and Heat Generation Calculation.

3.11. Assumptions Overview

1. The overall elliptical substrate cross-section that includes substrate and gas elements is estimated as square

2. The substrate material is cordierite

3. Temperature distribution within a single volume is homogeneous

4. The mass and thermal capacity of the washcoat are negligible

5. Axial conduction between gas elements is negligible

6. The flow is assumed fully developed and laminar

7. The pressure drop in the substrate is negligible

8. No gas is flowing in the gas volumes when the engine is turned off (i.e. internal convection is due to natural convection)

9. External convection is estimated as natural convection.

10. The engine-out exhaust is distributed evenly to every channel (i.e. there is no variation in gas velocity or species entering the gas volumes at the front face of the catalytic converter)

11. Exhaust hydrocarbons are represented by C₃H₈

12. Heat generation is primarily due to CO and C₃H₈ oxidation

The gas elements and their interactions with substrate elements are depicted in Figure 3.1-3.2. A single gas element, $T_{ijk}$, interacts with the surrounding substrate elements via a thermal resistance network including convection and conduction through the substrate. The gas elements also gain and lose energy through mass flow entering and exiting the element in the axial direction.

![Figure 3.1. Gas Element Thermal Network Cross-Sectional View](image1)

![Figure 3.2. Magnified View of Gas Element](image2)
The energy equation for a non-reacting flow applied to a gas element is expressed generally by:

$$\rho c_p \frac{dT}{dt} = \nabla \cdot (\dot{q} \cdot \hat{n})$$  \hspace{1cm} (3.1)

where

- $\rho$ is the density of the gas
- $c_p$ is the specific heat of the gas
- $T$ is the temperature of the gas at time, $t$
- $\dot{q}$ is the heat flux.

A numerical solution of Equation 3.1 can be obtained through an implicit forward-difference discretization and is expressed by Equation 3.2. Note that the expression was shortened through the ± notation in the subscript indices.

$$m_{gas} \rho_{gas} c_{p,gas} \frac{T_{i,j,k}^{t+1} - T_{i,j,k}^{n}}{\Delta t} = \frac{T_{i,j,k}^{t+1} - T_{i,j,k-1}^{t+1}}{R_{eq,gas}} + m_{gas} c_{p,gas} (T_{i,j,k}^{t+1} - T_{i,j,k}^{t})$$  \hspace{1cm} (3.2)

where

$$R_{eq,gas} = \frac{1}{h_{int} A} + \frac{L}{k_{wall} A}$$  \hspace{1cm} (3.3)

The mass, density, and specific heat of the gas inside a single element are represented by $m_{gas}$, $\rho_{gas}$, and $c_{p,gas}$ respectively. The heat transfer coefficient, $h_{int}$, was calculated using different correlations under engine running and engine off conditions. While the engine was running, the heat transfer coefficient was calculated from the Nusselt number.

$$h_{int} = \frac{Nu \cdot k_{gas}}{d_n}$$  \hspace{1cm} (3.4)

The Nusselt number correlation was obtained from Cengel et al. for laminar flow through a square channel with a uniform surface temperature:

$$Nu = 2.98$$  \hspace{1cm} (3.5)
The thermal conductivity’s, $k_{\text{gas}}$, dependence on temperature was estimated with a correlation from Ramanathan et al.

$$k_{\text{gas}} = 2.66 \times 10^{-4} \times T_{\text{gas}}^{0.805} \quad 3.6$$

Equation 3.6 provides $k_{\text{gas}}$ in SI units of [W/m/K] when the temperature is input in units of Kelvin.

The hydraulic diameter, $D_h$, for a square channel is:

$$D_h = \frac{4l^2}{4l} \quad 3.7$$

where

$l$ is the cross sectional length of the gas volume.

During engine off conditions Equation 3.2 can be reduced to Equation 3.8 by eliminating the mass flow term.

$$m_{\text{gas}}\rho_{\text{gas}}c_{p,\text{gas}} \frac{T_{i,j,k}^{t+1} - T_{i,j,k}^{t}}{\Delta t} = \frac{T_{i+1,j+1,k}^{t+1} - T_{i,j,k}^{t+1}}{R_{eq,\text{gas}}} \quad 3.8$$

For this condition, convection is estimated as free convection resulting in the convection coefficient:

$$h_{\text{int}} = h_{\text{int,free}} \quad 3.9$$


The substrate elements and thermal resistance networks are illustrated in Figures 3.3 and 3.4. A given substrate element interacts with gas elements as previously described, but also interacts with neighboring substrate elements.
The energy equation for the substrate element which interacts with the gas elements can be expressed by:

\[
\rho c_p \frac{\partial T}{\partial t} = \nabla (\bar{q} \cdot \bar{n}) + \dot{q}_{\text{gen}}
\]  

3.10
The heat generation that occurs on the washcoat surface is assumed to be lumped into the substrate element and included in Equation 3.10. However, it is neglected in the numerical solution to energy equation (Equation 3.11) and accounted for as later described.

\[
m_{sub} \rho_{sub} c_{p,sub} \frac{T_{i,j,k}^{n+1} - T_{i,j,k}^n}{\Delta t} = \frac{T_{i,j+1,k}^{n+1} - T_{i,j,k}^{n+1}}{R_{eq,sub}} + \frac{T_{i+1,j,k}^{n+1} - T_{i,j,k}^{n+1}}{R_{eq,sub}} + \frac{T_{i+1,j+1,k}^{n+1} - T_{i,j,k}^{n+1}}{R_{eq,gas}}
\]

where

\[
R_{eq,sub} = \frac{L}{k_{wall}A}
\]

The mass, density, and specific heat of the substrate element are represented by \( m_{sub} \), \( \rho_{sub} \), and \( c_{p,sub} \) respectively.

The outermost substrate elements interact with surface elements on the catalytic converter’s steel casing. The resulting thermal resistance is:

\[
R_{eq,sub-steel} = \frac{L}{k_{wall}A} + \frac{L}{k_{ins}A} + \frac{L}{k_{steel}A}
\]

Furthermore, the surface elements interact with the ambient surroundings through external convection. This results in the thermal resistance:

\[
R_{eq,air} = \frac{1}{h_{ext}A} + \frac{L}{k_{steel}A}
\]

where

\[
h_{ext} = h_{ext,free}
\]


Solving for heat generation is an iterative approach that involves solving species mass balance and reaction rate equations simultaneously. For this reason, it is calculated independently from the energy equations. The temperature increase corresponding to the rate of heat generation calculated at time, \( t \), is added to the current temperature array, \( [T^i] \), as indicated by Equation 3.10.
3.16. Since the chemical reactions are a surface phenomenon, the heat generation array only contains non-zero values for substrate elements; therefore, the gas elements are only indirectly affected by heat generation.

\[ [T^t]_{new} = [T^t] + \frac{\Delta t \cdot \dot{Q}_{gen}}{m_{sub} \rho_{sub} c_{p,sub}} \]  

Assembling the finite-difference equations representing the energy balance for all the elements leads to a system of equations that can be used to implicitly calculate the unsteady and spatially varying temperatures within the catalytic converter. The equations to calculate the temperature at a new time step, \( t+1 \), can be represented by:

\[ [T^{t+1}] = [M]^{-1} [T^t]_{new} \]  

where 

\( M \) is the matrix of temperature coefficients specific to individual elements.

3.15. Heat Generation Calculation

Before the aforementioned solution process can be completed, heat generation must be calculated by simultaneously solving the non-linear system of species mass balance and reaction rate equations. Those equations are developed in this subsection.

Species conservation is mathematically represented by:

\[ \frac{\partial C_i}{\partial t} = \nabla \cdot (D_i \nabla C_i) - \nabla \cdot (\vec{v}C_i) + R_i \]  

where

\( C_i \) is the concentration of species, \( i \)

\( R_i \) is the generation of species, \( i \) from the chemical reactions

\( D_i \) is the diffusion coefficient for species, \( i \)

\( \vec{v} \) is the velocity field
Two simplifications can be made when applying this to the stationary substrate element. First, flow velocities are non-existent in the assumed solid substrate material; therefore, the convection term is not significant. Secondly, since the reaction time scales are considerably shorter than diffusion of a given species, the quasi-steady assumption is applied thus eliminating the unsteady term. Applying these simplifications to Equation 3.18 gives:

\[ \nabla \cdot (D_i \nabla C_i) = -R_i \]  

3.19

Therefore, the overall reaction rates are controlled by the rate at which the reacting species diffuse from the gas to the substrate element where all the reactions are presumed to occur.

The quasi-steady assumption is also applied to the gas element species balance. Since no reactions occur there, the gas element species conservation becomes:

\[ \nabla \cdot (D_i \nabla C_i) = \nabla \cdot (\vec{v} C_i) \]  

3.20

Equations 3.19 and 3.20 can be equated and written in terms of species mole fractions, \( x_i \), rather than concentration, \( c_i \). Additionally, the molecular diffusion originally expressed with Fick’s Law can be represented with a diffusion mass transfer model analogous to Newton’s Law of Cooling in heat transfer resulting in:

\[
\frac{w}{A} \frac{\partial x_{g,i}}{\partial z} = -k_{m,i} S (x_{g,i} - x_{s,i}) = \sum_{j=1}^{3} a_j r_j s_{i,j} \tag{Ramanathan, 2011}
\]

3.21

where

- \( w \) is the total molar flow rate
- \( S \) is the ratio of the void cross-sectional area per unit volume of monolith
- \( A \) is the cross-sectional area of the gas element
- \( k_{m,i} \) is the diffusion mass transfer coefficient of a species from the gas element to the substrate element
$r_j$ is the reaction rate of reaction, $j$

$a_j$ is the catalyst surface area per unit volume of substrate

$s_{i,j}$ is the stoichiometric coefficient for species, $i$, of reaction, $j$

Two different mole fractions are denoted in Equation 3.21: the mole fraction of a species present in the gas element, $x_{g,i}$, and the mole fraction of a species adsorbed onto the substrate element, $x_{s,i}$. This mass and energy exchange between the gas and substrate elements is also depicted in Figure 3.5.
The mole fraction of a species in the substrate element, $x_{s,i}$, was assumed to be axially (z-direction) non-variant. This simplifies the differential equation to a simple, first-order equation with constant coefficients and an exponential solution. The resulting solutions are shown in Equations 3.22 and 3.23.

$$x_{g,i}(z) = c_1 e^{-A k_{m_j s_x} z} + x_{s,i}$$  \hspace{1cm} 3.22

$$x_{g,i}(z) = \frac{A z \sum_{j=1}^{\beta} a_j r_j s_{i,j}}{w} + c_1$$  \hspace{1cm} 3.23

Boundary Condition:

$$x_{g,i}(z = 0) = x_{g,i,engine\ out}$$  \hspace{1cm} 3.24

Therefore,

$$c_1 = x_{g,i,engine\ out}$$  \hspace{1cm} 3.25

Equations 3.22 and 3.23 can be developed for the gas elements at each axial division as shown in Equations 3.26 and 3.27. This helps to reduce the mathematical error presented by assuming $x_s$ as constant in the axial direction. Now, $x_s$ is only axially non-variant for a single element. Both Equations 3.26 and 3.27 are necessary in the solution process otherwise the system of non-linear equations would be undetermined.
\[ x_{g,i,i,j,k} = c_2 e^{-\frac{A k_{m,i} s_z}{w}} + x_{s,i,i,j,k} \]  \hspace{1cm} (3.26)

\[ x_{g,i,i,j,k} = \frac{A^2 \sum_{j=1}^3 a_{j} r_{j} s_{i,j}}{w} + c_2 \]  \hspace{1cm} (3.27)

where

\[ \tilde{z} = z - (k - 1) \Delta z \]

Boundary Condition:

\[ x_{g,i,j,k}(\tilde{z} = 0) = x_{g,i,i,j,k-1} \]  \hspace{1cm} (3.28)

Therefore,

\[ c_2 = x_{g,i,i,j,k-1} \]  \hspace{1cm} (3.29)

The expression for the mass transfer coefficient between the solid and gas elements, \( k_{m,i} \), was obtained from the Ramanathan et al. paper.

\[ k_{m,i} = \frac{S_h}{D_h} (c_g D_{l,m}) \]  \hspace{1cm} (3.30)

where

\[ c_g \] is the total gas concentration

\[ S_h = Nu = 2.98 \] (Ramanathan, 2011)  \hspace{1cm} (3.31)

The correlation for mass diffusivity, \( D_{l,m} \), was taken from Equation 11-4.4 of *The Properties of Gases and Liquids* and has units of cm²/s. The diffusivity volumes of the various gas species, \( \sum \) \( i \) were given in Table 11-1 of *The Properties of Gases and Liquids*. Note that \( \sum \) \( i \) represents a variable not a mathematical summation.

\[ c_g D_{l,m} = \left( \frac{0.00143 T_{gas}^{0.75}}{P^* \left( 2 \left( \frac{1}{M_i} + \frac{1}{M_N} \right)^{-1} \right)^{1/2} \left( \frac{3}{\sum T} + \frac{3}{\sum N} \right)^{1/2}} \right) \frac{P}{R_u T_{gas}} \]  \hspace{1cm} (3.32)
Table 3.1.

Diffusivity Volumes for Reactants and Products (Poling, 2007).

<table>
<thead>
<tr>
<th>i</th>
<th>Species, i</th>
<th>Diffusivity Volume, $\sum i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CO</td>
<td>18 cm$^3$</td>
</tr>
<tr>
<td>2</td>
<td>NO</td>
<td>4.54 + 6.11 cm$^3$</td>
</tr>
<tr>
<td>3</td>
<td>O$_2$</td>
<td>16.3 cm$^3$</td>
</tr>
<tr>
<td>4</td>
<td>C$_3$H$_8$</td>
<td>15.9<em>3 + 2.31</em>8 cm$^3$</td>
</tr>
<tr>
<td>5</td>
<td>N$_2$</td>
<td>18.5 cm$^3$</td>
</tr>
<tr>
<td>6</td>
<td>H$_2$O</td>
<td>13.1 cm$^3$</td>
</tr>
<tr>
<td>7</td>
<td>CO$_2$</td>
<td>26.9 cm$^3$</td>
</tr>
<tr>
<td>8</td>
<td>H$_2$</td>
<td>6.12 cm$^3$</td>
</tr>
</tbody>
</table>

The chemical reaction rate for a given species, $r_i$, is represented by a simplified three-equation reaction mechanism. The majority of heat generation in a catalytic converter is due to CO and unburned hydrocarbon (UHC) oxidation. An NO reduction reaction was also included so that NO conversion could be predicted. Therefore, the reactions modeled are limited to the reactions listed in Table 3.2. The corresponding reaction rate correlations and values of optimized kinetic parameters (Tables 3.3-3.4) were acquired from the Ramanathan et al. work. The surface reaction rates (Equations 3.31-3.33) are forms of the Arrhenius equations with units of moles per mole-sites per second.

Table 3.2.

Enthalpy of Reactions for Reactions used in Model (Ramanathan, 2011).

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Enthalpy of Reaction, $\Delta H_i$ (J/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_1$ CO + 0.5O$_2$ → CO$_2$</td>
<td>-2.83*10$^5$</td>
</tr>
<tr>
<td>$r_2$ C$_3$H$_8$ + 5O$_2$ → 3CO$_2$ + 4H$_2$O</td>
<td>-2.04*10$^6$</td>
</tr>
<tr>
<td>$r_3$ CO + NO → CO$_2$ + 0.5N$_2$</td>
<td>-3.73*10$^5$</td>
</tr>
</tbody>
</table>

$$r_1 = \frac{k_1 c_{s,CO} c_{s,O2} \exp \left( \frac{-E_i}{R g \gamma_{i,j,k}} \right)}{\sigma} \quad 3.33$$
\[ r_2 = \frac{k_2 C_{s,C3H8} C_{s,O2} \exp\left(\frac{-E_2}{R g T_{i,j,k}}\right)}{G} \]  \hspace{1cm} (3.34)

\[ r_3 = \frac{k_3 C_{s,CO} C_{s,NO} \exp\left(\frac{-E_3}{R g T_{i,j,k}}\right)}{G} \]  \hspace{1cm} (3.35)

where

\[ C_{s,i} = \left(\frac{P}{R_a T_{i,j,k}}\right) \chi_{s,i,j,k}^t \]  \hspace{1cm} (3.36)

Table 3.3.

Optimized Kinetic Parameters for Reactions Used in Model (Ramanathan, 2011).

<table>
<thead>
<tr>
<th>i</th>
<th>Optimized $k_i$</th>
<th>Optimized $E_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$5.542 \times 10^{13}$</td>
<td>121450</td>
</tr>
<tr>
<td>2</td>
<td>$6.404 \times 10^{15}$</td>
<td>165160</td>
</tr>
<tr>
<td>3</td>
<td>$2.857 \times 10^{9}$</td>
<td>52374</td>
</tr>
</tbody>
</table>

\[ G = \left(1 + K_1 C_{s,CO} + K_2 C_{s,C3H6}\right)^2 \left(1 + K_3 C_{s,CO}^2 C_{s,C3H6}^2\right) \left(1 + K_4 C_{s,NO}\right) \]  \hspace{1cm} (3.37)

where

\[ K_i = k_{i,G} \exp\left(\frac{-E_{LG}}{T_{i,j,k}}\right) \]  \hspace{1cm} (3.38)

The assumption was made that all of the hydrocarbons in the exhaust are represented by C$_3$H$_8$. Therefore, $C_{s,C3H6}$, which is present in Equation 3.37 is assumed to be zero.
Table 3.4.

Optimized Kinetic Parameters for Reactions Used in Model Continued (Ramanathan, 2011).

<table>
<thead>
<tr>
<th>i</th>
<th>Optimized $k_{i,G}$</th>
<th>Optimized $E_{i,G}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.314</td>
<td>-485</td>
</tr>
<tr>
<td>2</td>
<td>1.289</td>
<td>166</td>
</tr>
<tr>
<td>3</td>
<td>2.147 x 10^{-4}</td>
<td>-10163</td>
</tr>
<tr>
<td>4</td>
<td>8.699 x 10^5</td>
<td>3685</td>
</tr>
</tbody>
</table>

The reaction rates are converted to units of moles per m$^3$ per second by multiplying by the catalyst surface area per unit volume of substrate, $a_j$. The front catalyst loading ratio and total catalyst loading were unknown, so data for the GMT-900 catalytic converter (Ramanathan, 2011) was used for this work. Since there was no other evidence to assume otherwise, dispersion was estimated to be 100%.

$$a_j = \left(\frac{Loading_{Pt}}{Loading_{total}}\right) \times Loading_{cat} \times dispersion \times \left(\frac{1}{M_{Pt}}\right) + \left(\frac{Loading_{Pd}}{Loading_{total}}\right) \times Loading_{cat} \times dispersion \times \left(\frac{1}{M_{Pd}}\right) \times Loading_{cat} \times dispersion \times \left(\frac{1}{M_{Rh}}\right)$$

Equations 3.26-3.27 and 3.33-3.37 were assembled for each of the reactants in reactions listed in Table 3.2. MATLAB’s “fsolve” function was used to solve the system of non-linear equations. The “fsolve” non-linear equation solver utilizes a trust region algorithm and requires an initial guess for the variables for which it is solving. The viability of the solution was contingent on the initial guesses. The solver works by transforming the input equations into simplified, representative functions with a trust region that is dependent on the initial guess. If the minimum value of the function in this region is not within a certain tolerance of zero, no solution is found. Therefore, the values of the initial guesses require optimization.
The initial guess for the species entering the gas element was equivalent to the calculated value of the same species exiting the previous element:

\[ x_{g, in, i,j,k} = x_{g, out, i,j,k-1} \]  \hspace{1cm} (3.40)

The guesses for the mole fractions of NO, C\(_3\)H\(_8\), O\(_2\), and CO species exiting the element are guessed in terms of the mole fractions that entered the element:

\[ x_{g, NO, out, i,j,k} = \frac{i}{100} x_{g, NO, in, i,j,k} \]  \hspace{1cm} (3.41)
\[ x_{g, CO, out, i,j,k} = \frac{i}{100} x_{g, CO, in, i,j,k} \]  \hspace{1cm} (3.42)
\[ x_{g, C3H8, out, i,j,k} = \frac{i}{100} x_{g, C3H8, in, i,j,k} \]  \hspace{1cm} (3.43)
\[ x_{g, O2, out, i,j,k} = \frac{i}{100} x_{g, O2, in, i,j,k} \]  \hspace{1cm} (3.44)

where

\[ 0 < i < 100 \]

The initial guesses for the remaining variables being solved can be expressed in some way as the mole fractions entering and exiting a gas element. Therefore, the value of \( i \) is the only value to guess. Values of \( i \) between 90 and 99 produced optimal results.

Finally, heat generation was calculated for a substrate element with the iteratively calculated reaction rates:

\[ \dot{Q}_{gen} = -\sum_{j=1}^{\# \text{of rxns}} a_j \Delta H_j r_j \]  \hspace{1cm} (3.45)
Table 3.5.

Summary of Model Parameters Used as Inputs

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>(78% ethanol, 22% n-heptane)</td>
</tr>
<tr>
<td>Cordierite Density</td>
<td>2600 kg/m³</td>
</tr>
<tr>
<td>Cordierite Thermal Conductivity</td>
<td>4 W/m/K</td>
</tr>
<tr>
<td>Cordierite Specific Heat</td>
<td>1465 J/kg/K</td>
</tr>
<tr>
<td>Insulation Thermal Conductivity</td>
<td>0.2 W/m/K</td>
</tr>
<tr>
<td>Insulation Thickness</td>
<td>6 mm</td>
</tr>
<tr>
<td>Steel Thermal Conductivity</td>
<td>27.2 W/m/K</td>
</tr>
<tr>
<td>Steel Density</td>
<td>8050 kg/m³</td>
</tr>
<tr>
<td>Steel Thickness</td>
<td>3.175 mm</td>
</tr>
<tr>
<td>Steel Specific Heat</td>
<td>500 J/kg/K</td>
</tr>
<tr>
<td>Cat Loading</td>
<td>80 g/ft³</td>
</tr>
<tr>
<td>Platinum Loading</td>
<td>0</td>
</tr>
<tr>
<td>Palladium Loading</td>
<td>77.5/80</td>
</tr>
<tr>
<td>Rhodium Loading</td>
<td>2.5/80</td>
</tr>
<tr>
<td>Total Loading</td>
<td>Pt loading + Pd Loading + Rh Loading</td>
</tr>
<tr>
<td>Dispersion</td>
<td>100%</td>
</tr>
<tr>
<td>Internal Free Convection Coefficient</td>
<td>10 W/m²/K</td>
</tr>
<tr>
<td>External Free Convection Coefficient</td>
<td>10 W/m²/K</td>
</tr>
</tbody>
</table>

3.2. Experimental Setup

Experiments for model validation were conducted using an engine-dynamometer test bench which had emission measurement capability. The engine provided feedgas to a catalytic converter which was instrumented for temperature measurement. A standard five-gas emissions bench was used to sample the exhaust gas before and after the catalytic converter. Data were gathered using three distinct data acquisition (DAQ) systems. The interactions between those subsystems are shown in the full test cell schematic in Figure 3.6. Details on these systems are provided in the subsections that follow.
3.21. Engine-dynamometer

Experimental data were gathered using a GM 2.4 L LEA engine (Table 3.6) coupled to a 100 hp General Electric direct current (DC) electric dynamometer in the University of Alabama’s Engines and Combustion Laboratory (ECL).
Table 3.6.

2.4 L LEA Engine Specifications

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>88 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>98 mm</td>
</tr>
<tr>
<td>Displacement</td>
<td>2384 cc</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>11.2:1</td>
</tr>
<tr>
<td>Number of Cylinders</td>
<td>4</td>
</tr>
</tbody>
</table>

The key sub-systems which enable or influence the in-vehicle engine performance were replicated within the test cell to match their behavior in the vehicle. E85 was delivered by a fuel storage and delivery system that utilizes the controllers, pumps, sensors, and evaporative emissions control system present in the donor vehicle. The original LEA engine control module (ECM) was used for primary engine control. ECM I/O and communication with other vehicle controllers is emulated using a dSPACE hardware-in-the-loop (HIL) simulator and dSPACE Control Desk software. Speed control during experiments was achieved by manually entering speed commands via ethernet to the Inter-Loc V. Torque control was achieved by modulating accelerator pedal position (APP) signal voltage inputs transmitted to the ECM by the dSPACE HIL.

3.22. Exhaust Line Temperature Measurement

The exhaust system from the engine’s donor vehicle, a 2015 Chevrolet Equinox, was replicated up to and partially beyond the second catalytic converter. Locations of temperature measurements on the engine’s exhaust manifold and line are indicated in Figure 3.7.
The donor vehicle’s catalytic converter thermocouple instrumentation setup is pictured in Figures 3.9-3.10. The geometric parameters of the catalytic converter are shown in Table 3.7. Internal catalyst temperature measurement is obtained by an exposed-junction Omega Type K thermocouple probe. The probe is inserted into the catalyst brick one inch behind its leading edge in the center of the flow cross section. Surface temperature measurements are obtained from twisted junctions of Type K thermocouple wire. Junctions were placed at the smallest and largest radii of the catalytic converter cross-section, one inch behind the leading edge of the catalyst brick.
Table 3.7.

GM 2015 Chevrolet Equinox Catalytic Converter Geometry

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Minor Axis Radius</td>
<td>2.375 in</td>
</tr>
<tr>
<td>Major Axis Radius</td>
<td>3 in</td>
</tr>
<tr>
<td>Length</td>
<td>4 in</td>
</tr>
<tr>
<td>Cell Density, cpsi</td>
<td>1600</td>
</tr>
<tr>
<td>Wall Thickness</td>
<td>0.1 mm</td>
</tr>
</tbody>
</table>
The exhaust line’s thermocouple junctions were connected to a National Instruments (NI) cRIO 9022 Real-Time Controller-based DyneSystems DAQ box. The box’s thermocouple inputs were processed by an NI 9213 thermocouple cRIO card. The data obtained by the DyneSystems DAQ box were broadcast in real time on the ECL’s ethernet network. A custom NI LabView program then collected, processed, displayed, and recorded the real-time temperature measurement.

3.23. Emissions Measurement

Engine-out and post-catalytic converter 1 emissions were measured with a standard 5-gas emissions bench. The exhaust gas was not diluted and was transported in a heated line. Table 3.8 displays the exhaust species measured.
Table 3.8.

Species Measured with ECL’s 5-Gas Emissions Bench

<table>
<thead>
<tr>
<th>Measured Species</th>
<th>Measurement Type (Wet or Dry)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO, ppm</td>
<td>Dry</td>
</tr>
<tr>
<td>CO2, %</td>
<td>Dry</td>
</tr>
<tr>
<td>O2, %</td>
<td>Dry</td>
</tr>
<tr>
<td>C3H8, ppm</td>
<td>Wet</td>
</tr>
<tr>
<td>NO, ppm</td>
<td>Dry</td>
</tr>
</tbody>
</table>

Pre and post-catalytic converter emissions measurements for the species listed in Table 3.8 are shown in Figures A.1-A.10 in the Appendix.
CHAPTER 4
EXPERIMENTS FOR MODEL VALIDATION

Two test scenarios were performed to validate the catalytic converter thermal model: a warm-up and cool-down test. The scenarios were performed consecutively. Before a test, the catalytic converter and engine were allotted a 24-hour soak period (i.e. the engine was not operated for 24 hours). This was to ensure that there was no initial temperature gradient present in the catalytic converter and the ECM was commanding the engine to operate for cold-start conditions. An overview of the test conditions are shown in Tables 4.1-4.2.

Table 4.1.
Test Scenario 1: Engine Operating (Catalytic Converter Warm-up) Conditions

<table>
<thead>
<tr>
<th>Engine Speed</th>
<th>Engine Load</th>
<th>Ambient Temperature</th>
<th>Building Ventilation (on/off)</th>
<th>Fuel</th>
</tr>
</thead>
<tbody>
<tr>
<td>2500 rpm</td>
<td>40 lb-ft</td>
<td>24 C</td>
<td>off</td>
<td>E85 (78% alcohol, 22% gasoline)</td>
</tr>
</tbody>
</table>

Table 4.2.
Test Scenario 2: Engine Off (Catalytic Converter Cool-down) Conditions

<table>
<thead>
<tr>
<th>Engine Speed</th>
<th>Engine Load</th>
<th>Ambient Temperature</th>
<th>Building Ventilation (on/off)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 rpm</td>
<td>0 lb-ft</td>
<td>24 C</td>
<td>off</td>
</tr>
</tbody>
</table>
The engine speed and torque measurements through the duration of both tests are displayed in Figure 4.1.

![Engine Torque and Speed](image)

**Figure 4.1. Engine Torque and Speed for Test Scenarios 1 & 2**

Engine-out exhaust temperature is shown in Figure 4.2 There is a brief engine motoring period between the two tests and the effects of that are evident in the mid-catalytic converter temperature reading.
Pre and post-catalytic converter emissions measurements were made for model validation. The experimental setup was limited to obtaining emissions measurements one location at a time. Therefore, the measurements were obtained from two separate warm-up test runs. The engine speed and load were maintained constant for both runs, but slight differences in the catalytic converter’s warm-up behavior between the two tests is possible. The engine load for the pre and post-catalytic converter emissions measurement test runs are shown in Figures 4.3 and 4.4 respectively.
Air and fuel mass flow rates, temperature, and species concentrations measurements served as inputs to the model. Surface and mid-catalytic converter temperature as well as post-catalytic converter emissions measurements served as the key experimental data for model validation. Air and fuel mass flow rates (Figures 4.5 – 4.6) and fuel alcohol percentages were recorded from ECM CAN data using dSPACE Control Desk. The exhaust mass flow rate and
equivalence ratio (Figures 4.7 – 4.8) were calculated from air and fuel flow rates to use as a model input.

Figure 4.5. Intake Air Mass Flow Rate Measured in dSPACE

Figure 4.6. Fuel Mass Flow Rate Measured in dSPACE
The fuel alcohol percentage, mass flow rates, and emissions measurements were used to calculate the remaining engine-out species mole fractions by balancing the global chemical equation shown in Equation 4.1. These calculations were performed assuming n-heptane as an approximation for the hydrocarbon ratio of gasoline. Additionally, it was assumed that the only gases present in the exhaust other than the five measured were N$_2$, H$_2$, and H$_2$O.
The stoichiometric air to fuel ratio, $\alpha_{stoich}$, was calculated through balancing the chemical equation with the assumption of complete combustion.

\[ (1 - 0.78)C_7H_{16} + (0.78)C_2H_6O + \alpha_{stoich}(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + cN_2 \]  4.1

$N_2$, $H_2O$, and $H_2$ were solved by balancing:

\[ (1 - 0.78)C_7H_{16} + (0.78)C_2H_6O + \frac{\alpha_{stoich}}{\varphi}(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + cC_3H_8 + dCO + eO_2 + fNO + gH_2 + hN_2 \]  4.2

where

\[ \varphi = \alpha_{stoich} \times \frac{m_{fuel}}{m_{air}} \]  4.3
CHAPTER 5
RESULTS & DISCUSSION

The goal of any simulation is to achieve high accuracy with low computational time. Three approaches were taken in attempt to achieve this goal. The approaches and results of the optimal approach are discussed in this chapter.

Approach 1: The total volume of the substrate in the catalytic converter was maintained at its true value as the number of channels in the model were increased. The equation developed for the cross-sectional area of the gas flow element to keep the overall substrate volume at the true value is shown in Equation 5.1.

\[ a = \left( \frac{\sqrt{p \cdot R_{\text{major}} \cdot R_{\text{minor}}}}{\sqrt{\text{channels} + 1} + \sqrt{\text{channels}}} \right)^2 \]  

5.1

The wall thickness for a single substrate element is then calculated from Equation 5.2.

\[ t_{\text{wall}} = \frac{\sqrt{a}}{6} \]  

5.2

The mass flow rate of the gas entering a single channel in the model is calculated from the experimental exhaust mass flow rate and the total number of channels being modeled.

\[ \dot{m}_{\text{gas}} = \frac{\dot{m}_{\text{exhaust}}}{\text{channels}} \]  

5.3

Resultantly, as the number of channels were increased, the volumes of individual substrate and gas elements were reduced. The goal of this approach was to model as few channels as possible to achieve a gas channel volume to substrate volume ratio that produced
accurate temperature predictions. Unfortunately, the approach became too computationally expensive. For a computationally manageable number of channels, the relatively high wall thickness compared to the real substrate caused the substrate to under-predict warm-up time. In response, a second approach developed.

Approach 2: The wall thickness was maintained at its true value as the number of channels were varied.

\[ t_{wall} = 1 \text{ mm} \]  

5.4

The cross-sectional area of a single gas element is a function of the overall catalytic converter area, the defined wall thickness, and the number of channels being modeled as shown in Equation 5.5

\[ a = (\sqrt{\pi} \times R_{small} \times R_{large} - (\sqrt{\text{channels}} + 1) \times t_{wall})^2 \]  

5.5

\[ \dot{m}_{gas} = \frac{m_{exhaust}}{\text{channels}} \]  

5.6

This caused the model to severely under-predict mid-catalytic converter temperature because the large gas channel to substrate volume ratio caused too much heat transfer between the substrate and gas elements due to convection. Again, the appropriate number of channels needed to achieve a reasonable ratio compared to the true ratio was too computationally expensive.

Approach 3: The optimal approach was to model a miniature catalytic converter. In this case, the substrate and gas elements were the same size as the real catalytic converter, but the overall cross-sectional area of the catalytic converter was reduced. This allowed appropriate mid-catalytic converter temperature trends to be predicted during warm-up while modeling a small number of channels and therefore reduced computational time significantly. Unlike the first two
cases, the gas mass flow rate entering a single channel was based on the real number of channels as shown in Equation 5.7.

\[ m_{gas} = \frac{m_{exhaust}}{N} \]  \hspace{1cm} (5.7)

where

\( N \) is the number of channels for the real catalytic converter.

Since the miniature catalytic converter has significantly less channels than the real case, the remaining exhaust was assumed to not enter the catalytic converter.

5.1. Model Sensitivity & Results of Miniature Catalytic Converter Model (Approach 3)

MATLAB’s memory availability presented a significant limitation for this model. After model debugging, all unnecessary arrays that were created to save variables were removed. The model was still however limited by the size of the matrix of temperature coefficients. Despite the reduction in complexity by using the miniature catalytic converter approach, a relatively large amount of channels need to be modeled to accurately predict radial heat loss to the ambient surroundings. This is because the amount of channels determines the overall size of the modeled catalytic converter. The overall steel surface area to volume ratio increases with decreasing channels modeled. This causes an over-prediction of external convection for the miniature catalytic converter. Equation 5.8 was used to calculate the ratio of surface area/volume of the modeled case to the real case. The ratio as a function of channels modeled is shown in Figure 5.1. Based on this result, the estimated minimum number of channels that need to be modeled to obtain reasonable trends is 1600 channels and is identified in Figure 5.1.

\[
\left( \frac{Surface Area}{Volume} \right)_{model} / \left( \frac{Surface Area}{Volume} \right)_{real}
\]  \hspace{1cm} (5.8)
A minimum of 32 axial divisions was required for heat generation to be accurately predicted. Simulating 1600 channels and 32 axial divisions results in the creation of about 100,000 total elements. Modeling 100,000 elements creates a matrix of temperature coefficients that is beyond MATLAB’s memory capacity. Therefore, an adiabatic catalytic converter model was considered to analyze the model’s behavior. In the adiabatic model, there was no heat transfer between the outermost substrate elements and the steel surface and ambient surroundings. The adiabatic assumption is consistent with catalytic converter’s design. The catalytic converter is surrounded is by 6 mm of insulation to promote heat retention during warm-up for quick light-offs. The simulation results of the mid-catalytic converter temperature

Figure 5.1. Ratio of Catalytic Converter Surface Area/Volume of the Modeled Case to the Real Case
for the adiabatic model with 36 channels and 32 axial divisions is shown in Figure 5.2. Since warm-up predictions are overwhelmingly dependent on axial heat transfer, the lack of radial heat transfer due to the adiabatic assumption does not greatly affect warm-up trends. However, the majority of heat loss during real catalytic converter cool-down is due to radial heat transfer. Therefore, the only reduction of temperature during cool-down predicted by the adiabatic model is due to the brief engine motoring period.

![Figure 5.2. Adiabatic Model Mid-Catalytic Converter Temperature Predictions (36 channels x 32 axial divisions)](image-url)
Figure 5.3. Adiabatic Model Mid-Catalytic Converter Temperature Prediction for Warm-up Only (36 channels x 32 axial divisions)

The number of channels and axial divisions were varied as much as possible within MATLAB’s memory capacity in attempt to determine the model’s sensitivity during warm-up. The percent error for the cases modeled during the warm-up region are shown in Figure 5.4.
As expected, the number of channels and axial divisions (above 32) do not greatly affect accuracy for an adiabatic warm-up. This is a result of the correctly modeled substrate to gas element volume ratio. For the majority of warm-up, the adiabatic simulation temperature prediction produces error less than 3%. This result implies most of the heat transfer during warm-up is in the axial direction. This is expected because the real substrate is insulated for heat retention during warm-up.

The calibration ranges for the post-catalytic converter emissions measurements were not high enough to read maximum readings. Horizontal lines in the experimental emissions readings indicate the actual value was above the calibrated range. This effect is apparent in the
comparisons between simulation and experimental data for post-catalytic converter emissions shown in Figures 5.5-5.7. The simulated emissions before light-off are in correspondence with the pre-cat experimental data. The simulated C$_3$H$_8$ emissions trends correspond well with experimental data, but simulated CO emissions trends indicate the model is likely over-predicting CO oxidation rates during the light-off regime. This over-prediction could most likely be reduced by modeling more axial divisions, but again, the maximum amount of axial divisions were modeled for MATLAB’s memory capacity. Additionally, some error could be due to the pre-catalytic converter emissions measurements (served as a model input) being measured during a different test run than the post-catalytic converter emissions measurements. Despite the constant engine load between the two tests, there is always variability especially during engine testing. Overall, the simulation trends for the C$_3$H$_8$ and CO correspond decently with the experimental data. The simulated NO reduction happens faster than indicated by the post-cat experimental data, but errors in NO prediction have little effect on temperature prediction since the NO reduction reaction produces relatively low heat generation compared to the oxidation reactions.
Figure 5.5. Catalytic Converter-Out C$_3$H$_8$ Comparison
Figure 5.6. Catalytic Converter-Out CO Comparison
Figures 5.8-5.10 show modeled species conversion as a function of distance from the front face for varying times. By 35 seconds, all three reactions modeled reach peak conversion effectiveness by about one-fourth of the catalytic converter’s total length. In reality, species conversion cannot reach 100%. It’s expected that more realistic values (98-99% conversion effectiveness) could be predicted by modeling more axial divisions.
Figure 5.8. C₃H₈ Simulated Conversion Effectiveness
Figure 5.9. CO Simulated Conversion Effectiveness
Figure 5.10. NO Simulated Conversion Effectiveness
CHAPTER 6
CONCLUSIONS AND SUGGESTIONS FOR FUTURE WORK

The primary goal of this work was to develop and validate a 3-D catalytic converter model for future use as an engine on/off control strategy in a HEV supervisory controller. The primary conclusions and results are as follows:

- A miniature catalytic converter model was employed to meet MATLAB memory limitations.
- The miniature model alone was still unable to produce accurate trends of thermal behavior because it resulted in an over prediction of heat loss to the surroundings for the maximum channels that could be modeled within MATLAB’s memory preferences.
- An adiabatic assumption was made for the miniature model and allowed mid-catalytic converter temperature to be predicted with ± 3% error during warm-up.
- The adiabatic assumption prevents accurate cool-down temperature trends to be predicted because radial conduction is the primary mode of heat transfer during cool-down.

Warm-up predictions from the adiabatic simulation indicate the model is physically correct. Since the target supervisory controller is modeled in MathWorks Simulink, MATLAB was the ideal platform for the thermal model. However, MATLAB proved to be an improper tool
for a model of this complexity, and the code should be ported to a more robust programming language. Another option would be to non-dimensionalize parameters such that external convection heat transfer can be predicted for the miniature catalytic converter model.

Once the model is fully validated, it can be used either independently or in conjunction with Simulink to develop the engine on/off control strategies. Independently, the model works by importing engine speed and torque for the duration of a drive cycle. As of now, the model requires engine-out exhaust temperature and emissions as an input. However, either predictions of those values or maps could be used with decent accuracy. The model would report mid-catalytic converter temperature prediction (or any temperature in the catalytic converter) for the duration of the simulated drive cycle. Based on those results, the engine control strategy could be adjusted. Ideally, the model would work conjunctly with Simulink. Since the analytical model exists as a source code, a function that contains the source code could be imported into Simulink. If computational time is reduced enough, the model can serve as a real time control strategy in determining whether or not the engine should be on or off based on if the catalytic converter temperature/effectiveness.
REFERENCES


“General Motors Believes it has the Answer to the Automotive Air Pollution Problem.” (1974, September 11). Toledo Blade, p. 62.


Figure A.1. Experimental Pre-catalytic Converter CO Emissions
Figure A.2. Experimental Pre-catalytic Converter CO$_2$ Emissions
Figure A.3. Experimental Pre-catalytic Converter \( \text{C}_3\text{H}_8 \) Emissions
Figure A.4. Experimental Pre-catalytic Converter NO Emissions
Figure A.5. Experimental Pre-catalytic Converter O₂ Emissions
Figure A.6. Experimental Post-catalytic Converter CO Emissions
Figure A.7. Experimental Post-catalytic Converter CO$_2$ Emissions
Figure A.8. Experimental Post-catalytic Converter $C_3H_8$ Emissions
Figure A.9. Experimental Post-catalytic Converter NO Emissions
Figure A.10. Experimental Post-catalytic Converter O\textsubscript{2} Emissions