

Vehicle and Drive Cycle Simulation of a Vacuum Insulated Catalytic Converter

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ABSTRACT

A GT-SUITE vehicle-aftertreatment model has been developed to examine the cold-start emissions reduction capabilities of a Vacuum Insulated Catalytic Converter (VICC). This converter features a thermal management system to maintain the catalyst monolith above its light-off temperature between trips so that most of a vehicle's cold-start exhaust emissions are avoided. The VICC thermal management system uses vacuum insulation around the monoliths. To further boost its heat retention capacity, a metal phase-change material (PCM) is packaged between the monoliths and vacuum insulation. To prevent overheating of the converter during periods of long, heavy engine use, a few grams of metal hydride charged with hydrogen are attached to the hot side of the vacuum insulation.

The GT-SUITE model successfully incorporated the transient heat transfer effects of the PCM using the effective heat capacity method. A variety of conventional, stop-start and hybrid electric vehicles have been simulated over standard drive cycles using this model. For each vehicle, prep-cycle simulations were followed by soak simulations of differing time periods. Model predictions show that the VICC was able to maintain converter temperatures above 300°C for at least 12 hours for all of the simulated vehicles and standard prep-cycles. Furthermore, this heat retention ability directly translated to a proportional reduction in cold-start exhaust emissions. With the introduction of intermediate soak times as part of the EPA emissions test regulations, the benefits of the VICC should be seen in all standard drive cycle emissions tests. The simulation results of the GT-SUITE model demonstrate the contribution of the Vacuum Insulated Catalytic Converter in meeting stringent future emission standards.

CITATION: Daya, R., Hoard, J., Chanda, S., and Singh, M., "Vehicle and Drive Cycle Simulation of a Vacuum Insulated Catalytic Converter," *SAE Int. J. Engines* 9(3):2016, doi:10.4271/2016-01-0967.

INTRODUCTION

The industrial revolution of the 19th century was perhaps the most significant period in recent human history. However, the benefits in productivity and life standard came with a cost; an exponential rise in emitted pollutants from anthropogenic sources. One of the key sources of these emissions was the automobile. Automobile emissions can be broadly classified into four categories: carbon monoxide (CO), unburned hydrocarbons (HC), oxides of nitrogen (NO_x) and particulates (PM) [1]. It is important to differentiate these four forms of emissions from carbon dioxide (CO₂). While CO₂ is produced in large quantities from any form of fuel combustion, it is not a toxic pollutant. However, it is a greenhouse gas and is increasingly being subjected to stringent regulations, especially in Europe. The drive to control all these emissions began with the enactment of the first emissions regulation by California in 1959, and there has been a progressive reduction in the statutory limits for tailpipe emissions [1, 2]. Furthermore, it has been shown in [3] that for the average drive distance (trip distance) of real-life traffic, nearly all of the CO and

HC exhaust emissions for gasoline engines occur during the cold-start phase. Therefore, lowering cold-start emissions has become the primary focus of industry emissions control development efforts [2].

Since tailpipe emissions are inversely related to converter temperature, several techniques have attempted to promote catalyst light-off by supplying heat. The most common way is to retard combustion timing, increasing the exhaust heat flux rate at the expense of fuel consumption [4]. Other techniques, like the electrically heated converter (EHC) and fuel-fired burner systems [3], require some form of power input, and possibly increase the parasitic losses from the engine. One of the most important alternatives in this regard is the Vacuum Insulated Catalytic Converter (VICC). This technology uses vacuum insulation, metal bellows, radiation shields and phase-change material (PCM) to keep the converter above light-off temperature following long periods of cold-soak. Vacuum insulation prevents convective and radiative heat loss from the substrate to the ambient. Metal bellows near the inlet and outlet of

the VICC attempt to significantly increase the axial conduction heat flow path, and therefore reduce conduction losses from the substrate. Finally, the space in between the catalyst brick and vacuum insulation is packed with phase-change material (PCM). The PCM exchanges energy with the substrate as it melts and solidifies. As a result, it acts as a thermal accumulator, and stores some of the thermal energy present in the exhaust gases. This energy is used to keep the converter warm during vehicle soak.

The VICC was originally developed at the National Renewable Energy Laboratory (NREL), a U.S. Department of Energy (DOE) national laboratory [6, 7], and featured a metal eutectic alloy phase-change material (PCM) with a melting temperature of 575°C. Although limited Federal Test Procedure (FTP) emission testing failed to fully melt the PCM, noticeable drive-cycle emission reductions were observed. Further testing and analysis by NREL and Benteler Automotive [8, 9] demonstrated the heat retention capacity of the VICC, with NMHC and CO emissions reductions of 66% and 65% respectively. However, another set of vehicle tests using ceramic monoliths [10] questioned the ability of the VICC to fully melt the PCM during real-world driving cycles, and therefore its ability to achieve significant cold-start emissions reductions.

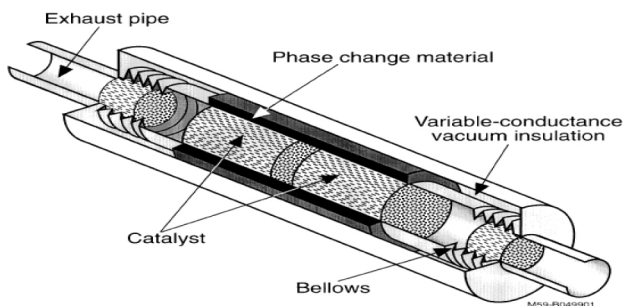


Figure 1. Major features of the vacuum-insulated catalytic converter [9].

In this paper, a VICC-type converter has been modeled and simulated in GT-SUITE. This aftertreatment model simulated drive cycle runs followed by long periods of vehicle soak. A vehicle-aftertreatment model was also developed to simulate the VICC for a variety of drive cycles, ambient conditions and vehicle types. This model used steady-state engine-out maps to provide the required inputs for the exhaust system model. Hybrid Electric Vehicles (HEVs) represent an important field of application for the VICC, since they experience periods of engine shut and catalyst cooldown during vehicle operation. Thus, a HEV-aftertreatment model was also developed and simulated to analyze the benefits of the VICC. Finally, the VICC was simulated on drive cycles representing real-world driving behavior. Driving data from the 2010-12 California Household Travel Survey has been processed by NREL [11] to obtain speed vs time plots representative of real-world drive cycles. This simulation is an attempt to emphasize the ability of the VICC to achieve real-world cold-start emissions reductions.

COLD-START CONVERTER MODELING

The VICC was modeled using GT-SUITE v7.5 build 3, the latest available version of the software. Initially, a standalone aftertreatment model was developed comprising of the exhaust system only. This model used second-by-second engine-out emissions and temperature data as input.

Transient Aftertreatment Model

A detailed description of the TWC catalyst modeling (except the vacuum insulation and PCM) and the governing equations used to numerically solve for model parameters is given in the GT-SUITE Aftertreatment Manual [12]. The GT-SUITE model of the VICC was divided into three sections: Sections I and III consisted of the pipe and cone before and after the catalyst substrates, and Section II was composed of two stainless-steel catalyst substrates placed in series. A 3 ft. main takedown pipe was connected to Section I of the VICC, and Section III of the VICC was connected to a 3 ft. tailpipe. An overview of the GTSUITE model is shown in Figure 2.

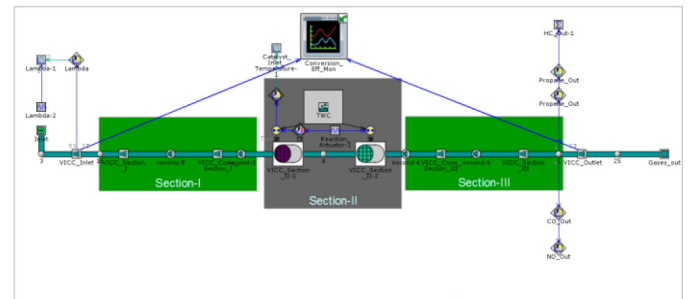


Figure 2. GT-SUITE aftertreatment model of the VICC

Section-I and Section-III

The dimensions of the stainless-steel pipe and cone elements were determined through careful measurement of the prototype converter. Additionally, the thermal properties of the vacuum layer were considered to be extremely low (thermal mass $\approx 1e-7$ J/m³-K), but not zero. This was for model stability considerations. Due to the non-uniformity of the outer layers in the prototype, an equivalent average thickness was calculated for the model. Few details of the dimensions used in the model are listed in Table 1.

Table 1. VICC Section-I and Section-III Specifications

Pipe Length	16 mm
Pipe Diameter	6 mm
Cone Length	4.32 mm
Cone Diameter	6 cm-9.6 mm
Stainless Steel Layer Thickness	0.1651 mm
Equivalent Vacuum Layer Thickness above Pipe	2.936 mm
Equivalent Vacuum Layer Thickness above Cone	3.31 mm

Open orifices are used in GT-SUITE to connect any two flow components, and they can either be conducting or nonconducting. Metallic bellows were not modeled explicitly due to their complex geometry. Instead, the reduction in conduction heat loss was modeled using a “no-conduction” orifice between the pipe and cone elements.

Section-II

Section-II consisted of two metallic substrates arranged in series. This type of arrangement can allow for using two different substrates for optimal light-off time and conversion efficiencies. However, in the simulation results presented in this paper, both catalyst substrates were modeled identically with the same reaction kinetics. The substrates were surrounded by two outer layers comprising of stainless steel and phase-change material (PCM). The PCM used for the present simulation was a Magnesium-Zinc-Aluminum (Mg-Zn-Al) metal eutectic alloy. The density and specific heat of the PCM were evaluated using individual element properties and mass fractions, and the thermal conductivity was taken from [13]. The latent heat capacity of the PCM (L) was modeled implicitly by incorporating it with the specific heat capacity (c_p) into an effective heat capacity (c_{eff}) using

$$c_{eff} = \frac{L}{T_2 - T_1} + c_p$$

where T_1 is the temperature at which melting or solidification begins and T_2 is the temperature at which the material is fully melted or solidified [14]. This prevented the need for an elaborate control system that transferred heat to or from the catalyst substrate when part of the PCM reached melting temperature. Some details about the substrate dimensions and the PCM thermal properties are listed in Table 2.

Table 2. VICC Section II Specifications

Channel geometry	Square
Diameter	9.6 mm
Length (each of 2)	11.8 mm
Cell density	78 cells/cm ²
PGM loading	3.4 g/L
PCM mass	3.9057 kg
PCM Latent Heat	236.609 kJ/kg
PCM melting temperature	339°C-340°C
PCM solid phase density	2776 kg/m ³
PCM liquid phase density	2561 kg/m ³
PCM solid phase specific heat	715 J/kg-K
PCM liquid phase specific heat	957 J/kg-K

The heat transfer through the catalyst substrate wall was modeled using a 2-D conduction object that considered both axial and radial temperature gradients in the substrate. Ten radial sub-volumes and forty axial sub-volumes were used for each substrate. However, due to limitations in the present version of GT-SUITE, this 2-D conduction approach meant the distinct outer layers of the converter would be lumped together into one layer with effective thermal

properties. As a result, due to its extremely low thermal mass, the vacuum insulation layer above the substrates was not modeled explicitly. Instead, its effect was modeled as a significant reduction in the external heat transfer coefficient. This form of modeling assumed a near perfect insulation with very little heat flow through the vacuum layer.

An example template was used to model the three-way catalyst (TWC) reaction mechanism. A reaction actuator was used to turn off all the reactions during vehicle soak. Sensors were used to monitor the conversion efficiencies for CO, HC and NO_x, and compare them with temperature. Finally, tailpipe emissions were sensed in g/s. The basic reaction mechanism is shown in Figure 3. More details about the development and validity of this reaction mechanism can be found in [15].

Associated Site Element	Reactants	Products	Pre-exponent Multiplier	Temperature Exponent	Activation Temperature or Energy
PGM ...	CO+0.5O2 ...	CO2 ...	5.542E13 ...	0 ...	121450 ...
PGM ...	C3H6+4.5O2 ...	3CO2+3H2O ...	1.917E15 ...	0 ...	129530 ...
PGM ...	C3H8+5O2 ...	3CO2+4H2O ...	6.404E15 ...	0 ...	165160 ...
PGM ...	H2+0.5O2 ...	H2O ...	1.814E15 ...	0 ...	111450 ...
PGM ...	CO+NO ...	CO2+0.5N2 ...	2.857E9 ...	0 ...	52374 ...
PGM ...	C3H6+9NO ...	3CO2+3H2O+4.5N2 ...	2.994E11 ...	0 ...	80063 ...
PGM ...	H2+NO ...	H2O+0.5N2 ...	7.88E10 ...	0 ...	69237 ...
PGM ...	CO+H2O ...	CO2+H2 ...	180000 ...	0 ...	56720 ...
PGM ...	C3H6+3H2O ...	3CO+6H2 ...	123000 ...	0 ...	81920 ...
cerium ...	2Ce2O3+O2 ...	4CeO2 ...	2.943 ...	0 ...	5296 ...
cerium ...	Ce2O3+NO ...	2CeO2+0.5N2 ...	792 ...	0 ...	25101 ...
cerium ...	CO+2CeO2 ...	Ce2O3+CO2 ...	0.1824 ...	0 ...	31768 ...
cerium ...	C3H6+12CeO2 ...	6Ce2O3+3CO+3H2O ...	13.57 ...	0 ...	39070 ...
cerium ...	C3H8+14CeO2 ...	7Ce2O3+3CO+4H2O ...	17.7 ...	0 ...	39680 ...
cerium ...	H2+2CeO2 ...	Ce2O3+H2O ...	2.845 ...	0 ...	31768 ...

Figure 3. TWC Ramanathan and Sharma reaction mechanism [15]

In order to understand the relative benefits of the VICC, a conventional converter (CC) aftertreatment model was developed as a control case. This model had the same features as the VICC model with the same dimensions for the flow elements. However, it did not have any outer layer vacuum insulation or PCM. Additionally, this model had the option to choose between a ceramic (cordierite) and metal monolith. The ceramic monolith was wrapped with an intumescent mat outer layer. The dimensions and thermal properties of this mat were representative of a Unifrax XPE-AV2 ®, and were obtained by directly contacting the supplier.

Table 3. Substrate Specifications

Metal substrate thickness	0.05 mm
Ceramic substrate thickness	0.15 mm
Intumescent Mat thickness	5.8 mm
Alumina washcoat thickness	0.03 mm

Several assumptions were made in the model development to simplify the analysis while capturing the key heat transfer effects:

1. Metallic bellows present in the prototype to increase the conduction heat path were modeled as straight pipes.
2. The dimensional change of the phase-change material (PCM) on melting/solidification was not considered.
3. The thermal properties of the PCM were assumed to undergo a step change during melting/solidification.

- The copper foil radiation shield was modeled implicitly as a reduction in the surface emissivity of the stainless-steel material above which it was present (from 0.1 to 0.05 for simplicity).
- Uniform precious metal loading assumed with no gas-phase reactions in the substrate.

Steady-State Vehicle-Aftertreatment Model

In addition to a standalone transient aftertreatment model, vehicle-aftertreatment models were developed to analyze the VICC over different drive cycles and ambient conditions. Since the aftertreatment system was identical to the standalone transient model, all of the assumptions mentioned for that model were also applicable to the vehicle-aftertreatment model. The fundamental difference between the two models was the engine-out emissions and temperature input form. While the transient model relied on second-by-second data over an FTP, the steady-state model calculated these inputs using engine maps. A detailed engine model for combustion was not developed as this would require further validation, and would deviate from the principal goals of the research.

Conventional and Stop-Start Vehicles

In simulations of vehicles for driving cycle fuel economy and emissions, it is sometimes convenient to directly impose the state (typically speed) of a node on the driveline. For an energy balance to be satisfied at all times, this requires allowing a source or sink of power, and the torque or force associated with this source, to “float” and be solved for by this simulation. In GT-SUITE, the term *kinematic analysis* is used to describe these types of simulations [16].

A default GT-SUITE vehicle model was chosen as a starting point for the model development. This model used an imposed drive cycle vehicle speed to back calculate engine speed and load, a method known as *backward kinematic analysis*. It also consisted of a simple engine-state model with mechanical output, fuel consumption and friction maps. More details about this type of simulation can be found in the GT-SUITE Vehicle Manual [16].

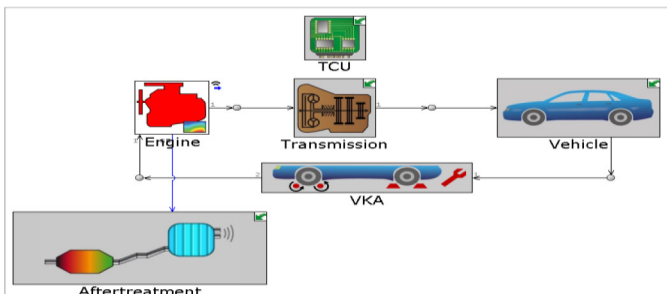


Figure 4. GT-SUITE vehicle-aftertreatment model for conventional and stop-start vehicles

The engine-state component was modified to introduce the appropriate fuel properties and steady-state maps. For stop-start vehicle simulations, the engine-state was reconfigured to introduce

fuel shutoff. No modifications were made to the 4-gear automatic transmission or the transmission control unit (TCU). Some details of transmission specifications are shown in Figure 5.

Attribute	Unit	Gear #1	Gear #2	Gear #3	Gear #4
Gear Ratio		2.393...	1.45...	1...	0.677...
In-Gear Efficiency		1...	1...	1...	1...
Friction Torque	N-m	ign...	ign...	ign...	ign...
Input Moment of Inertia	kg-m ²	0.0025...	0.0025...	0.0025...	0.0025...
Output Moment of Inertia	kg-m ²	0.0025...	0.0025...	0.0025...	0.0025...
Gear Ratio Transition Time	s	0.5...	0.5...	0.5...	0.5...
Gear Ratio Transition Up		def...	def...	def...	def...
Gear Ratio Transition Down		def...	def...	def...	def...
Input Torque Multiplier for Clutched Shifting		def (=0.0)...	def (=0.0)...	def (=0.0)...	def (=0.0)...
Dissipated Fraction of Upshifting Energy		def (=0.0)...	def (=0.0)...	def (=0.0)...	def (=0.0)...
Gear Input Torque Limit	N-m	ign...	ign...	ign...	ign...

Figure 5. Specifications of the 4-speed automatic transmission used in the vehicle-aftertreatment model

The vehicle sub-assembly was used to specify dimensional and tire specifications for the vehicle chosen for simulation. The vehicle specifications used in the model (shown in Figure 6) were representative of 2015 Ford Taurus. The drive-cycle speed (in km/hr) was imposed using the vehicle kinematic analysis (VKA) object. This imposed speed was used to evaluate the engine speed and brake torque, and therefore estimate the engine-out emissions and exhaust gas temperature using emissions and temperature maps. The exhaust gas flow rates in the engine maps were tabulated in kg/hr, and these were converted to mass fractions before being fed into the aftertreatment system.

Vehicle Mass	lb	4035...
Passenger and Cargo Mass	kg	136...
Vehicle Drag Coefficient		0.29...
Vehicle Frontal Area	m ²	2.7...
Vehicle Wheelbase	in	112.9...
Horizontal Dist From Last Rear Axle to Mass Center	in	56.45...
Nominal Tire Width	mm	245
Aspect Ratio	%	45
Diameter of Wheel	in	20
Rolling Radius Speed Dependence Correction	fraction	0.97
Tire Rolling Resistance Factor		0.008
Tire Inflation Pressure	bar	ign
Friction Coefficient Limit		0.7

Figure 6. Vehicle specifications used in GT-SUITE Model

Hybrid Electric Vehicles

As mentioned earlier, hybrid electric vehicles (HEVs) represent a significant area of application for the VICC. During electric mode operation, most HEVs experience converter cooldown. Sometimes, it might be even be necessary to keep the engine running to prevent the converter from falling below light-off temperature. With the introduction of the VICC, this additional engine operation can be avoided, and could lead to fuel consumption benefits along with reduction in emissions.

To analyze the VICC for HEVs, a HEV-aftertreatment model was developed using GT-SUITE. Typically in HEV simulations, it is more convenient to calculate a power demand to follow the speed target because of the various, and often complex, HEV configurations. In